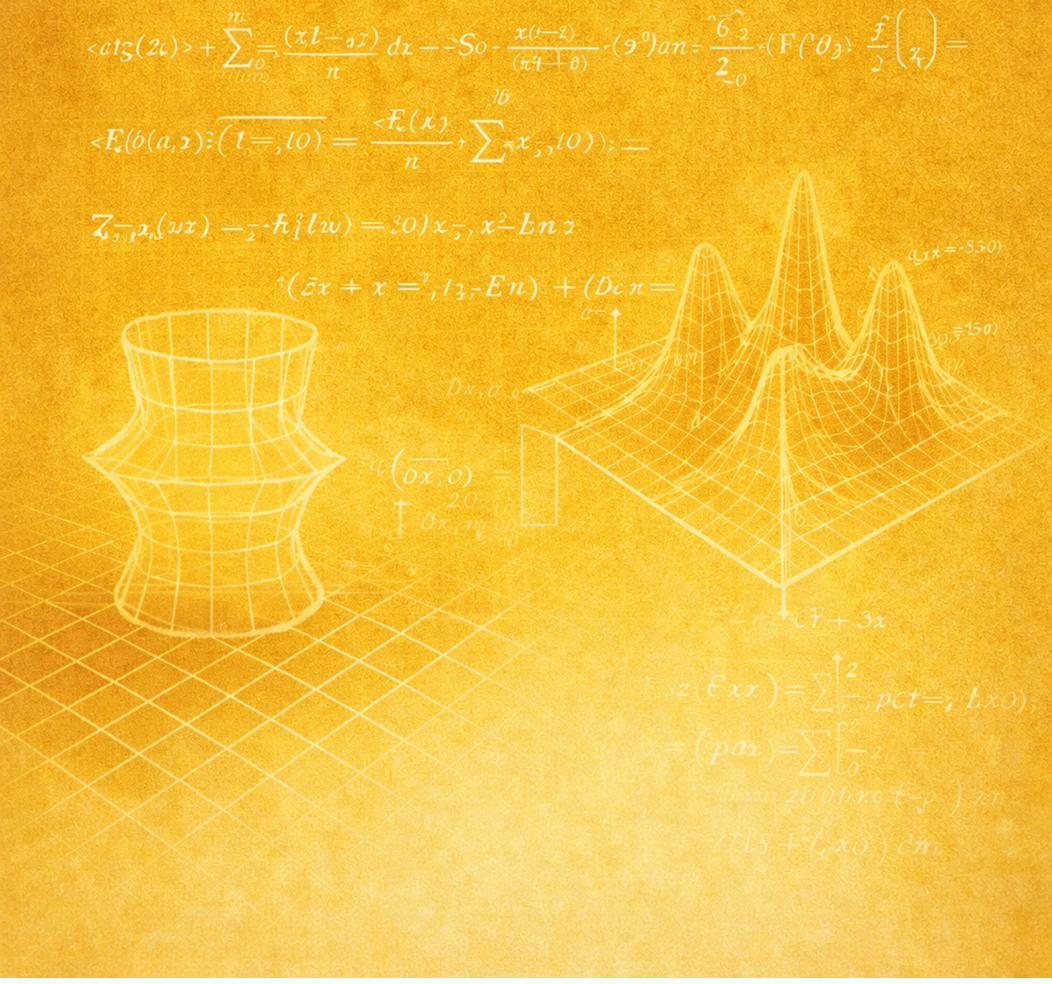
V.L. Bonch-Bruevich
& S.V. Tyablikov

THE GREEN FUNCTION METHOD in STATISTICAL MECHANICS



V.L. Bonch-Bruevich
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Translated from the Russian and edited by
D. TER HAAR, *Clarendon Laboratory, Oxford*

THE GREEN FUNCTION METHOD IN STATISTICAL MECHANICS

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Foreword by N. N. BOGOLYUBOV

1962

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FOREWORD

The main problem of quantum mechanical as well as of classical statistical mechanics is the many-body problem. It consists essentially of finding effective methods for evaluating equilibrium and non-equilibrium characteristics of systems containing an extremely large number of particles. Recently new possibilities have appeared which are connected with a systematic use of quantum field theoretical methods. One of the most effective among these is apparently the method of the time- and temperature-dependent Green functions which are the natural developments of the tools developed first of all in connexion with problems in quantum electrodynamics and meson physics. The use of "dynamical" Green functions which are defined as averages over the ground state of the system turned out already to be very effective for solving several problems in statistical physics. However, only the generalisation to the case of finite temperatures which combined quantum field theoretical ideas with density matrix methods made it possible to reveal the power of this method.

The logical developments in statistical mechanics in recent years were such that the method of temperature-dependent Green functions was initially developed simultaneously at a number of institutes both in the Soviet Union and abroad. These developments were very intensive and in many directions. Apart from a study of general problems the method was also extensively applied to solve specific problems.

The present monograph discusses both basic ideas and applications of the Green function method. It does not cover everything because there is such a wide field to cover; it is mainly based upon the investigations of the authors themselves. It is the first attempt at a systematic statement of this class of problems and of several applications to plasmas, ferromagnetism, superconductivity, and related problems.

One may expect that this monograph will turn out to be useful for all who wish to master the Green function method or to study different specific results.

Academician N. N. Bogolyubov

AUTHORS' PREFACE

The present monograph is devoted to a new method for solving many-body problems: the so-called quantum-mechanical Green function method. A great number of papers devoted to this method have appeared in recent years. We do not attempt to cover all of these: this monograph is essentially based upon our own work. The list of references does not pretend to be complete: we have referred mainly to those papers which are related to the text. We emphasise the general method. Chapters I to III are devoted to this; they contain the general spectral theory of the non-relativistic temperature-dependent Green functions depending on two time arguments. We establish in these chapters the connexion between the Green functions and the thermodynamic and kinetic characteristics of a system.

Chapters IV to VII are devoted to illustrating the method and to applying it to different problems in the physics of condensed media: the theory of electron plasmas in solids, electron-phonon interactions, ferromagnetism at finite temperatures. We were the first to obtain a number of the results given in these chapters and we hope that they may be of interest by themselves. In the appendices we have given some information which it is desirable to know for an understanding of this book, but which has not been assumed to be known beforehand.

This book is intended for those who know the basic theory of quantum mechanics and statistical mechanics; in particular, density matrix methods and second quantisation are assumed to be known. Some results from quantum field theory which are used are formulated in the appendices.

The authors express their sincere gratitude to Academician N. N. Bogolyubov for pointing out to them the possibilities of the Green function method for statistical problems and for many discussions of problems arising in this connexion. His constant interest in this project has been an inestimable help to us.

B. V. Medvedev kindly looked through appendices I and III and made some very valuable suggestions for which we are sincerely grateful.

We are very grateful to Sh. M. Kogan and V. A. Moskalenko for reading through the manuscript and making some valuable suggestions for improvements in the presentation, and also to Yu. V. Gulyaev and A. G. Mironov for a careful examination of the first three chapters of the manuscript.

We finally express our sincere gratitude to A. A. Gusev for

carefully going through the manuscript and making several improvements in it.

Moscow, 16 December 1959

V. L. Bonch-Bruevich
S. V. Tyablikov

FOREWORD TO THE ENGLISH EDITION

The method of quantum Green's functions is being developed so quickly that it is almost impossible to publish a fully up to date book. Therefore the authors can but regret the absence of some interesting results in the book, but can propose no remedy to this except of writing a new one.

The authors should like to express their deep appreciation to Professor D. ter Haar who undertook the laborious task of translating the book and was kind enough to write the addendum.

V. L. Bonch-Bruevich
S. V. Tyablikov

TRANSLATOR'S PREFACE

The present translation of this monograph on the so-called Green function method differs in a few respects from the Russian original. The authors kindly provided me with some additional material, notably in sections 2 and 3, which has been incorporated. I should like to express my thanks to them for making this material available for the English edition. Moreover, a number of misprints have been corrected, in a few places a footnote has been added, and an index has been provided. The main difference between the translation and the Russian original consists in appendix VII which is a very brief survey of developments which occurred after the Russian manuscript was sent to the publishers in 1959. This survey is of necessity brief and is not meant to cover these developments exhaustively or in detail, but merely to provide the reader with some idea of how fruitful the Green function method has turned out to be and with a list of references for further study. It is hoped that this extra appendix will further increase the usefulness of this important addition to the many-body theory literature.

Oxford, March 1962 D. ter Haar

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INTRODUCTION

The method of the quantum-mechanical Green functions combines the most effective techniques of modern quantum field theory (Schwinger 1951a, b) with the concept of a chain of "particle" distribution functions which has been used for a long time in statistical physics (Bogolyubov 1947). Such a combination is apparently the best way to solve the essential difficulties which occur when one attempts to consider dynamically a many-body system in statistical mechanics *. The difficulties just mentioned are not just specific for a few specially chosen physical systems, but are general for this whole class of problems. They are connected with the characteristic singularity of statistical systems: the macroscopically large number of degrees of freedom **. The macroscopically large dimensions of the system have as a consequence that its total energy (both in the ground state and in excited states) turns out to be proportional to the volume V. The differences between different energy levels of the system (in particular, the values of the "excitation energies" which are the energy differences between the excited states and the ground state) depend as a rule only very little on the volume and are, generally, completely independent of the volume in the limit as $V \to \infty$ ***. In most problems where one studies the physics of a condensed medium one is just interested in the asymptotic behaviour of the energies of the excitations in the limit as $V \to \infty$. It is under those circumstances clearly very risky to endeavour to determine the energies of the excitations which are simply the differences of two large numbers (which increase without bound as $V \to \infty$). From this follows the requirement which must be satisfied by any method for solving the many-body problem in statistical physics: the spectrum of the excitation energies must be determined directly from some property of the eigenvalues which is asymptotically (as $V \to \infty$) independent of the volume. We shall see in sections 4 and 5 that if one uses the

* Here and in the following we consider, of course, the problem of a system of many interacting particles. The difficulties mentioned here do not occur in the trivial case of a perfect gas, when one can solve the dynamical problem exactly.

** This is the basis of the close mathematical kinship of the problems of statistical physics and those of quantum field theory. Indeed, in the latter one always deals with systems of an infinite number of degrees of freedom. In this sense any problem in relativistic quantum field theory is a many-body problem.

*** This limit is taken here and henceforth in the usual sense: $V \to \infty$, $N \to \infty$ (N: number of particles), while $N/V = n$ = constant.

spectral properties of the Green functions this requirement is automatically satisfied; this is the first advantage of the method discussed here.

Moreover, the fact that the total energy, the thermodynamic potential, and so on, are proportional to the total volume of the system makes it possible to introduce the corresponding specific quantities which will then be asymptotically independent of the volume. It are usually just those quantities which are of most interest and their evaluation is one of the important theoretical problems. Mathematically this leads to the evaluation of the ratio of two quantities which simultaneously increase without limit. Attempting to solve this problem directly can lead to well-known complications. Accordingly there arises yet another requirement of any method of solving the statistical many-body problem: such a method must ensure a clear-cut distinction between extensive and intensive quantities. We emphasise that this is a far from trivial problem. It is well known, for instance, that when one attempts to evaluate directly the ground state energy using standard quantum-mechanical perturbation theory methods there may occur terms which contain "non-physical" higher powers of the volume. Although it is clear from the beginning that when one sums the perturbation theory series these terms must cancel one another, it is far from simple to prove this. Moreover, the presence of terms depending on arbitrarily high powers of the volume leads to an exceptionally bad convergence of the perturbation series (if it converges at all). Van Hove (1955, 1956) and Hugenholtz (1957) have in this connexion developed a special form of perturbation theory which ensures a separation of terms containing different powers of V in a separate group. We shall see in section 12 that in the Green function method the distinction of intensive and extensive quantities occurs automatically: another advantage.

An important feature of many-body systems is the possibility of the occurrence of excited states of a special kind which are caused by the interparticle interactions and which thus have no counterpart in the case of a perfect gas (a classical example of such excitations are the plasma oscillations in a gas discharge or in a solid). Since the interaction causes here not simply adjustments in the free particle energies but states of an essentially new character, an important theoretical problem is to create a method which enables us to look for the appearance of new branches in the energy spectrum *. We shall shew in sections 4, 5, and 11 that if we use the spectral properties of the Green functions this problem is also solved: a third advantage of this method.

Closely connected with the different branches of the energy spec-

* We emphasise that we are not discussing here whether the interactions are strong or weak, but the fact that these branches of the energy spectrum of the system may not occur at all when there are no interactions.

trum is the question of the elementary excitations of the system, the "quasi-particles"; a perfect gas of these quasi-particles imitates in the well-known sense the behaviour of free particles while at the same time it describes low-lying excitations of a many-body system. This representation which during the last twenty years has served as the basis for the theoretical discussion of a number of problems in the physics of condensed media has up to now all the same not been built upon a sufficiently general foundation. The Green function method gives apparently a final solution of this problem while at the same time also exposing the limits of the applicability of the concept of elementary excitations.

Let us in this connexion note the following facts:

First of all, the representation of a "quasi-particle" character of some of the branches of the energy spectrum of a many-body system occurs in the theory without introducing any special assumptions whatever. It follows in its general form from the spectral theorems of sections 3 to 5 which connect the singularities of the Green functions with the quantities which determine the evolution in time of the system. These theorems are valid under very general assumptions and the foundation given here of the idea of elementary excitations is thus not connected with any approximation and is a final solution in that sense.

Secondly, it follows from the same spectral theorems that, generally speaking, the number of quasi-particles is not an integral of motion (the wave functions of states with a given number of quasi-particles are, generally speaking, not harmonic functions of the time, but are damped).

In other words, a perfect gas of quasi-particles does not describe truly stationary, but only quasi-stationary states of the system, and one can only use this representation provided the damping is sufficiently small, that is, provided the line width is small compared to the excitation energies per particle. In that sense the concept of elementary excitations is an approximate one, and the method of evaluation determines automatically the limits of its applicability, because it enables us to determine the damping constants. One must, however, emphasise that one practically always in the statistical physics of condensed media deals with these quasi-particle states. Indeed, concepts such as mean free path or mean free time of flight have only a meaning in such a case. The reason for this is that (if there are interparticle interactions) it is impossible to eliminate completely the exchange of energy, momentum, and so on, between different degrees of freedom. The tacitly admitted neglect of the fact that the states are non-stationary when one evaluates thermodynamic quantities is just another approximation which is valid under the above mentioned conditions (weak damping). The introduction of elementary excitations with a finite life-time does, of course, not alter the situation, but only expresses it in the clearest possible way.

Thirdly, and finally, the so-called quasi-particle energies turn out to be, generally speaking, temperature-dependent (section 16). This circumstance is not astonishing as the quasi-particle spectrum is defined through quantities which characterise the evolution in time of a mixture (with a Gibbs probability distribution of different "pure" states initially). The problem of "temperature-dependent energy levels" is often discussed in the literature. We wish to emphasise in this connexion that it is first of all necessary to define exactly what one means by this term. The Green function method gives apparently the clearest answer to this problem.

One of the most important and at the same time one of the most difficult problems in statistical physics is the study of phase transitions. We shall study specific examples in chapters VI and VII and shall see that the Green function method gives a well-known possibility to approach a solution of this problem also.

An important advantage of the Green function method is, finally, that it enables us to solve by the same method problems of a very different nature and moreover both equilibrium and transport problems. This last circumstance is especially important for us. It is well known that for a number of solid state problems the standard method of applying the transport equation meets with great difficulties, both calculational (anisotropic systems) and of a more essential nature (systems with a short time of free flight and in a strong magnetic field). A large number of papers has in recent years been devoted to attempts to go beyond the frame work of the transport equation. We shall shew in sections 14 and 15 that the Green function method gives apparently the most natural formal apparatus to solve transport problems.

The first application of the Green function method to problems of non-relativistic solid state theory (at $T = 0$) was in 1954 (Bonch-Bruevich 1955a, 1956a) in a paper written on the initiative and suggestion of N. N. Bogolyubov. In the further development an important part was played by the spectral theorems of Källen (1952) and Lehmann (1954) which were obtained in connexion with quantum field theory problems. Transferring them to the case of the non-relativistic solid state theory (Bonch-Bruevich 1956b) enabled us to establish in a general form the connexion between the singularities of the Green functions and the characteristics of the energy spectrum of the system considered. The Green function method was thereafter developed by a number of authors (Galitskiĭ and Migdal 1958, Galitskiĭ 1958, Gor'kov 1958, Belyaev 1958a, b, Migdal 1957, 1958, Klein and Prange 1958, Prange and Klein 1958, Abrikosov and Gor'kov 1958) in connexion with different statistical problems. In all papers just quoted the discussion was, however, restricted to the case $T = 0$, and this made it difficult to use the methods which were developed to study the thermodynamic properties of a system. Matsubara (1956) was the first to attempt to produce a method which was

suitable for non-vanishing temperatures; in his paper he considered, however, only time-independent Green functions which did not make it possible for him to apply them to a study of energy spectra of the systems considered. A complete generalisation of the method to arbitrary temperatures was then soon worked out (Bonch-Bruevich and Kogan 1959, 1960, Kogan 1959, 1960, Bogolyubov and Tyablikov 1959, Bonch-Bruevich 1959a, Landau 1958a,b, Fradkin 1959, Abrikosov, Gor'kov, and Dzyaloshinskiĭ, 1959, Martin and Schwinger 1959).

We shall mainly consider non-relativistic many-body problems, explicitly writing down separately the time-coordinates. Relativistic notations and relations are used only when we formulate the problem of a system of particles with electro-magnetic interactions, since it leads to a simpler way of writing down the equations and makes some proofs easier. Even in that case, however, we bear in mind the subsequent non-relativistic approximation (for the particles).

The notation in this book is mainly the conventional one. The symbols a^+ and a denote both fermion- and boson- second-quantisation operators when fields are quantised, the number of particles of which are conserved. We use the notation ξ^+ and ξ for the creation and annihilation operators of the phonon field, the electromagnetic field, and similar fields. Time variables are denoted by $x_0, x_0', \ldots$ The symbol x denotes, depending on the context, either the set $\{\lambda, x_0\}$ where λ are some dynamical variables (λ-representation), or, in a particular case, the set $\{\vec{x}, x_0\}$ where $\vec{x}$ represents the spatial position coordinates. For the four-dimensional Fourier integral we use the rule

$$f(x) = \int \mathrm{d}^4k \; \mathrm{e}^{-\mathrm{i}kx} f(k) \; , \qquad f(k) = \frac{1}{(2\pi)^4} \int \mathrm{d}^4x \; \mathrm{e}^{\mathrm{i}kx} f(x) \; .$$

Here $kx = k_0 x_0 - (\vec{k} \cdot \vec{x})$, $\mathrm{d}^4k = \mathrm{d}^3\vec{k} \, \mathrm{d}k_0$, $\mathrm{d}^4x = \mathrm{d}^3\vec{x} \, \mathrm{d}x_0$.

Roman vector indices always take on the values 1, 2, and 3, and Greek indices the values 0, 1, 2, and 3. The metrical tensor $g_{\alpha\beta}$ which occurs in relativistic formulae is of the form

$$g_{\alpha\beta} = g^{\alpha\beta} \; , \qquad g_{00} = - g_{11} = - g_{22} = - g_{33} = 1 \; ;$$

$$g_{\alpha\beta} = 0 \; , \qquad \text{if} \qquad \alpha \neq \beta \; .$$

The commutators and anti-commutators are denoted, respectively, by $[\ldots]_-$ and $[\ldots]_+$.

The symbol Trace denotes the sume of the diagonal elements of a matrix in the second-quantisation representation, and the symbol Tr denotes the trace only with respect of the spin-indices. Unless a statement is made to the contrary summation over repeated spinor or tensor indices is always understood to be implied.

We assume always that charges and currents have a sign.

We use Heaviside units and units where $\hbar = 1$. The final formulae

in chapters IV to VII are, however, also written in the usual Gaussian system of units.

The superscript + indicates the Hermitean conjugate, or the complex conjugate.

Chapter I

BASIC RELATIONS

1. THE DENSITY MATRIX AND TIME-CORRELATION FUNCTIONS

The most complete way to describe an arbitrary quantum-mechanical system is by means of the density matrix (or statistical operator) ρ. The matrix elements of ρ can be written in the form (see Von Neumann 1955, Bogolyubov 1949, ter Haar 1961a)

$$(\lambda \mid \rho \mid \lambda') = \sum_n W_n \, \Phi_n(\lambda_1, \ldots, \lambda_N, t) \, \Phi_n^+(\lambda_1', \ldots, \lambda_N', t) \quad (\sum_n W_n = 1) \, . \tag{1.1}$$

Here N is the number of particles in the system, $\lambda_1, \ldots, \lambda_N$ are variables on which the eigenfunctions Φ_n of the total Hamiltonian depend (they could, for instance, be the $3N$ spatial coordinates - or the $3N$ momentum components - and N spin indices, if we were dealing with a system of N particles), n numbers the state described by the function Φ_n; $0 < W_n < 1$ (the number W_n is usually interpreted as the probability that the n-th state is realised), and t is the time.

Once we know the explicit form of the density matrix we can in principle evaluate the average value $\widetilde{F}$ of any dynamic variable, F, using the formula

$$\widetilde{F} = \text{Trace } \rho \, F \equiv \langle F \rangle \, . \tag{1.2}$$

The averaging is here (and henceforth everywhere) understood in both the purely quantum-mechanical and in the statistical sense. In particular, if the system is in statistical equilibrium and if the temperature T tends to zero, the right hand side of (1.2) goes over into the usual formula for the quantum-mechanical average (expectation) value. It is well known (Von Neumann 1955) that the equation of motion for ρ is of the form

$$i \frac{\partial \rho}{\partial t} = H \rho - \rho H \, , \tag{1.3}$$

where H is the total Hamiltonian of the system. We shall not discuss here in detail the problem of the boundary conditions applicable to (1.3) as its solution does not enter into our problems. We remind ourselves merely that for statistical equilibrium we get for ρ the expression for a grand ensemble:

$$\rho = C \, e^{-\beta H + \beta \mu N} \, , \tag{1.4}$$

where $\beta = (k_B T)^{-1}$ (k_B: Boltzmann's constant), μ is the chemical potential per particle, N the operator of the total number of particles in the system, and C a normalising constant which is usually written in the form

$$C = e^{\beta\Omega} .$$

The quantity Ω is a thermodynamic potential with as independent variables μ and T and is determined from the normalisation condition

$$\text{Trace } \rho = 1 . \tag{1.5}$$

From (1.5) and (1.4) we get

$$\Omega = -\frac{1}{\beta} \ln \text{Trace } e^{-\beta H + \beta\mu N} . \tag{1.6}$$

When we consider a system of identical particles we must take into account that the operators H and N in (1.4) act only in the function space which is of the necessary symmetry - symmetric or antisymmetric with respect of a permutation of the arguments - depending on the statistics which the particles in the system under consideration satisfy.

The density matrix ρ is, however, always symmetric with respect to a permutation of "particles", that is, when we perform simultaneously the same permutation of the arguments in each of the products $\Phi_n \Phi_n^+$ occurring in (1.1).

We emphasise that it is very important for us that we use a grand ensemble as we shall in the following often have to work with operators which do not conserve the number of particles. It is therefore convenient for us to introduce a "generalised Hamiltonian"

$$H' = H - \mu N . \tag{1.7}$$

The quantity μ occurs everywhere as a parameter to be determined from the condition that the number of particles in the system is a constant. If we talk in the following about stationary states of the system we shall have in mind eigenvalues and eigenfunctions of the operator (1.7).

We note that the parameter μ occurring in (1.7) is only the same as the chemical potential occurring in (1.4) if the operator H does not contain a term cN, where c is a constant. In the opposite case the chemical potential is then equal to the sum $\mu + c$. One can, however, always get rid of the term cN by a suitable choice of the zero energy. By analogy with the renormalised mass in quantum field theory this procedure is sometimes called the renormalisation of the chemical potential. We shall in the following assume that μ is the already renormalised chemical potential.

Equations (1.1) to (1.6) contain essentially the whole thermodynamics and all transport properties of any given system. If we exclude the case of a perfect gas which is of little interest, the direct

use of these equations is, however, accompanied with extraordinary difficulties. First of all, it is usually just as difficult to solve (1.3) (in a non-stationary case) as it is to solve the Schrödinger equation for a many-body system. Secondly, a just as difficult problem is often the evaluation of the trace (1.2) even, if the density matrix is known.

Fortunately, if we want to solve a particular problem, in the majority of cases we do not, in fact, need all the information contained in the density matrix (Bogolyubov 1947, 1949). Indeed, practically always one is only interested in operators of a single- or two-particle type. If we evaluate the average of dynamic variables described by these operators, the general formula (1.2) is considerably simplified.

Let us as an example consider an additive operator A; we shall shew that its average value $\tilde{A}$ for a system of N identical particles is given by the expression

$$\tilde{A} = \text{Trace}\, A\ \rho_1\ , \tag{1.8}$$

where ρ_1 is obtained by taking the trace of $N\rho$ over all variables $\lambda_1, \ldots, \lambda_N, \lambda_1', \ldots, \lambda_N'$ bar one pair:

$$(\lambda_1 | \rho_1 | \lambda_1') = \operatorname*{Trace}_{(2,\ldots,N)} N\rho(1,\ldots,N)\ . \tag{1.8a}$$

Indeed, if A is an additive operator, we can write it in the form

$$A = \sum_{r=1}^{N} A(\lambda_r, \lambda_r') \equiv \sum_{r=1}^{N} A(r)\ .$$

Its average value is given by

$$\tilde{A} = \sum_{r=1}^{N} \text{Trace}\, A(r)\ \rho\ .$$

By virtue of the symmetry of ρ with respect to a permutation of the particle arguments the value of Trace $A(r)\ \rho$ will be independent of r and we have thus

$$\tilde{A} = N \operatorname*{Trace}_{(1,2,\ldots,N)} A(1)\ \rho \equiv \operatorname*{Trace}_{(1)} A(1) \operatorname*{Trace}_{(2,\ldots,N)} N\rho\ .$$

One sees easily that this expression is the same as the one obtained by substituting (1.8a) into (1.8).

It has been shewn by Bogolyubov (1949) that it is convenient to write the expression for ρ_1 in the second-quantisation representation. To do this we introduce a complete orthonormal set of functions which depend on the variables λ of one particle: $\{\varphi_f(\lambda)\}$. We can then write A in the form

$$A = \sum_{f_1, f_1'} A(f_1, f_1')\ a_{f_1}^{+}\ a_{f_1'}\ .$$

We shall also assume that ρ is given in the second-quantisation representation:

$$\rho = \rho(\ldots, n_{f'}, \ldots; \ldots, n_f, \ldots) .$$

We get then for the average $\tilde{A}$

$$\tilde{A} = \sum_{f_1, f_1'} A(f_1, f_1') \underset{\{\ldots, n_f, \ldots\}}{\text{Trace}} a_{f_1}^+ a_{f_1'} \rho .$$

The trace in this equation is, however, nothing but the statistical average of $a_{f_1}^+ a_{f_1'}$:

$$\langle a_{f_1}^+ a_{f_1'} \rangle = \underset{\{\ldots, n_f, \ldots\}}{\text{Trace}} a_{f_1}^+ a_{f_1'} \rho =$$

$$= \sum_{\substack{\ldots, n_f, \ldots \\ \ldots, n_{f'}, \ldots}} (a_{f_1}^+ a_{f_1'}) \ldots, n_f, \ldots; \ldots, n_{f'}, \ldots \rho(\ldots, n_{f'}, \ldots; \ldots, n_f, \ldots) .$$

and we get for $\tilde{A}$

$$\tilde{A} = \sum_{f, f'} A(f, f') \langle a_f^+ a_{f'} \rangle .$$

Comparing this expression with (1. 8) we see that

$$(f | \rho_1 | f') = \langle a_f^+ a_{f'} \rangle . \tag{1.9}$$

We can now easily change over to the λ-representation, and we find

$$(\lambda | \rho_1 | \lambda') = \sum_{f, f'} \langle a_f^+ a_{f'} \rangle \varphi_f^+(\lambda) \varphi_{f'}(\lambda') = \langle a_\lambda^+ a_{\lambda'} \rangle . \tag{1.9a}$$

We shall call ρ_1 the "single-particle" (or first) density matrix. To avoid misunderstandings we emphasise that the term "single-particle" does not by any means imply a neglect of interparticle interactions. It only indicates the number of arguments on which ρ_1 depends. Completely analogously we get for the average value of any pair-operator B the equation

$$\tilde{B} = \tfrac{1}{2} \text{ Trace } B\rho_2 . \tag{1.10}$$

The matrix elements of the operator ρ_2 are given by the equation

$$(\lambda_1, \lambda_2 | \rho_2 | \lambda_2', \lambda_1') = \langle a^+(\lambda_1') a^+(\lambda_2') a(\lambda_2) a(\lambda_1) \rangle . \tag{1.11}$$

We shall call ρ_2 the "two-particle" (second, pair-) density matrix.

By analogy with (1. 9) and (1. 10) we can introduce "s-particle" density matrices with matrix elements

$$(\lambda_1, \ldots, \lambda_s | \rho_s | \lambda_s', \ldots, \lambda_1') = \langle a^+(\lambda_1') \ldots a^+(\lambda_s') a(\lambda_s) \ldots a(\lambda_1) \rangle , \tag{1.12}$$

which are only necessary to evaluate averages of s-particle opera-

tors. The operators ρ_s are for finite s asymptotically independent of V as $V \to \infty$ (Bogolyubov 1949).

In practice it is only necessary to know ρ_1 and ρ_2 to solve most problems in statistical physics, and one does not need at all the complete density matrix ρ. The question arises of course whether it would not be possible to determine ρ_1 and ρ_2 directly without beforehand evaluating the complete density matrix ρ (that is, in particular, without solving the Schrödinger equation of a system of interacting particles). One might expect that this problem would turn out to be appreciably simpler than an attempt to evaluate ρ directly, if only because the number of arguments of the functions to be determined is now smaller. This was the problem put by Bogolyubov (1947, 1949) who obtained a set of equations for the functions ρ_1, ρ_2, ... We must note that because of the interparticle interactions this set of equations is, generally speaking, an infinite chain of coupled equations including ρ_s of higher and higher order. The basic difficulty of this problem is the necessity to find some kind of "decoupling" of this set of equations; at this point one usually introduces various approximations.

We note that apart from ρ_1 and ρ_2 we are also interested in functions depending on two time coordinates, the so-called time-correlation functions, for instance,

$$(\lambda_1, \ldots, \lambda_s \,|\, \rho_s(t,t') \,|\, \lambda_s', \ldots, \lambda_1') = \langle a^+(\lambda_1', t') \ldots a^+(\lambda_s', t') a(\lambda_s, t) \ldots a(\lambda_1, t) \rangle . \quad (1.13)$$

As $t' \to t$, (1.13) goes over into (1.12). "Double-time" averages such as (1.13) play an important role in transport problems as they describe the evolution in time of the system. Indeed, let us first of all consider the case $T = 0$. The right hand side of (1.13) then becomes a quantum-mechanical average of the ground state of the system:

$$(\Phi_0, a^+(\lambda_1', t') \ldots a^+(\lambda_s', t') a(\lambda_s, t) \ldots a(\lambda_1, t) \Phi_0) , \quad (1.14)$$

where Φ_0 is the ground state wavefunction. It is clear that one can interpret the quantity (1.14) for $t < t'$ as the (unnormalised) probability amplitude for finding the state $a(\lambda_s', t') \ldots a(\lambda_1', t') \Phi_0$ at time t', if we had at time t the state $a(\lambda_s, t) \ldots a(\lambda_1, t) \Phi_0$ (since these states are, generally speaking, non-stationary states, this quantity decreases in absolute magnitude as $t' - t \to \infty$). At finite temperature ($T \neq 0$) the quantities (1.13) describe the evolution of a mixture.

One can, finally, also introduce "many-time" correlation functions where each a- and a^+-operator has its own time argument, but we have not had any need for those so far. We note also that one often meets with other combinations of operators, for instance, expressions of the kind

$$<a^+(\lambda_1',t')a(\lambda_1,t')a^+(\lambda_2',t)a(\lambda_2,t)>$$

(see sections 5 and 12). We shall see in the following that quantities of this kind are just the ones which determine, for instance, transport coefficients (electrical conductivity, and so on).

To simplify the notation we shall denote by $C_1(x)$ and $C_2(x')$ any product of a- and a^+-operators; x denotes here both the time ($t = x_0$) and the λ; in particular, λ may denote the usual coordinate vector ($\vec{x}$) or the momentum vector ($\vec{p}$). Similarly, x' denotes the time ($t' = x_0' \neq x_0$, in general) and the variables λ' (which are of the same kind as the λ). In accordance with our earlier discussion our problem will be a study of the quantities

$$K(x,x') = <C_1(x)C_2(x')> . \tag{1.15}$$

We note the important special case where $C_2 = C_1^+$, $x_0 > x_0'$, and $T = 0$. The right hand side of (1.15) is then, apart from a multiplying factor, the probability amplitude of finding at time x the state $C_1^+(x)\Phi_0$, if the system at time x_0' were in the state $C_1^+\Phi_0$. In particular, if $\lambda' = \lambda$, the function $K(\lambda,x_0;\lambda,x_0')$ describes the evolution in time of the state $C_1^+(\lambda,x_0)\Phi_0$. As before, if $T \neq 0$, we must talk about the evolution of a mixture.

In the following we shall only be interested in the case of statistical equilibrium when the operator ρ is given by (1.4).

2. THE SPECTRAL REPRESENTATION OF A SIMPLE PRODUCT

It is clear that for statistical equilibrium $K(x,x')$ can depend only on the time difference $x_0 - x_0' = t$, and that we can thus write $K(x,x') = K(\lambda,\lambda';t)$ as a simple Fourier integral. This way of writing K we shall call its spectral representation. We shall see that the corresponding Fourier transform possesses important properties which we shall widely use for specific applications in the following.

We shall denote by Φ_n and E_n the eigenfunctions and eigenvalues of the generalised Hamiltonian H' given by (1.7). The index n stands here for a set of quantum numbers which completely determine the state Φ_n. We introduce the notation

$$p_n = e^{\beta\Omega - \beta E_n} . \tag{2.1}$$

We can then write (1.15) in the form

$$\begin{aligned} K(x,x') &= \sum_n p_n(\Phi_n, C_1(x)C_2(x')\Phi_n) \\ &= \sum_{n,n'} p_n(\Phi_n, C_1(x)\Phi_{n'})(\Phi_{n'}, C_2(x')\Phi_n) , \end{aligned} \tag{2.2}$$

if we use the fact that the set of functions Φ_n is a complete one. The

sums in (2.2) may include integrals over continuous variables n. We note that although in the product $C_1 C_2$ we are only interested in that part of it which conserves the number of particles (if this is not the case, the averaging process in (1.15) leads to a vanishing result), the operators C_1 and C_2 may not conserve the number of particles separately (this happens, for instance, in the important case when $C_1 = C_2^+ = a(\lambda, t)$). The representation (2.2) (and also the spectral representation (2.5) following from it) has thus, generally speaking, a meaning only for systems with a varying number of particles. This is the reason why we take averages over grand ensembles.

We use now the equation of motion for the operators C_1 and C_2:

$$\frac{\partial C_j}{\partial x_0} = \mathrm{i}\,(H'\,C_j - C_j\,H')\,, \qquad j = 1, 2\,. \tag{2.3}$$

Because of (2.3) we get

$$\begin{aligned}(\Phi_n, C_1(x)\Phi_{n'}) &= (\Phi_n, C_1(\lambda, x_0{=}0)\Phi_{n'})\, e^{+\mathrm{i}(E_n - E_{n'})x_0}\,,\\ (\Phi_{n'}, C_2(x')\Phi_n) &= (\Phi_{n'}, C_2(\lambda', x_0'{=}0)\Phi_n)\, e^{-\mathrm{i}(E_n - E_{n'})x_0}\,.\end{aligned} \tag{2.4}$$

We define the spectral function $J(\lambda, \lambda'; E)$ by the equation

$$J(\lambda, \lambda'; E) = \sum_{n,n'} p_n \delta(E - E_{n'} + E_n)(\Phi_n, C_1(\lambda, x_0{=}0)\Phi_{n'})(\Phi_{n'}, C_2(\lambda', x_0{=}0)\Phi_n)\,. \tag{2.5}$$

We then get from (2.2) and (2.4) ($t = x_0 - x_0'$)

$$K(x,x') \equiv K(\lambda, \lambda'; t) = \langle C_1(x) C_2(x')\rangle = \int_{-\infty}^{+\infty} \mathrm{d}E\; e^{-\mathrm{i}Et} J(\lambda, \lambda'; E)\,, \tag{2.6}$$

and similarly

$$K'(x,x') \equiv K'(\lambda, \lambda', t) = \langle C_2(x') C_1(x)\rangle = \int_{-\infty}^{+\infty} \mathrm{d}E\; e^{-\mathrm{i}Et - \beta E}\; J(\lambda, \lambda'; E)\,. \tag{2.7}$$

If we now put $t = 0$, we get expressions for the ensemble averages

$$\begin{aligned}\langle C_1(\lambda, x_0) C_2(\lambda', x_0)\rangle &= \int_{-\infty}^{+\infty} \mathrm{d}E\; J(\lambda, \lambda'; E)\,,\\ \langle C_2(\lambda', x_0) C_1(\lambda, x_0)\rangle &= \int_{-\infty}^{+\infty} \mathrm{d}E\; e^{-\beta E}\; J(\lambda, \lambda'; E)\,.\end{aligned} \tag{2.8}$$

Equations (2.6) to (2.8) reduce the problem of evaluating the equilibrium and non-equilibrium characteristics of a system to the determination of the corresponding spectral functions. In the final reckoning this is what makes the Green function method effective, since we shall see in the following sections that one can immediately express the spectral functions in terms of Green functions.

It follows from (2.6) and (2.7) that the spectral functions for the products of two operators taken in different order (C_1C_2 and C_2C_1) differ from one another by a factor $e^{-\beta E}$. It follows from this, in particular, that if the two operators commute or anticommute with one another (for $x_0' = x_0$), the following identity holds

$$\int_{-\infty}^{+\infty} dE\, J(\lambda, \lambda'; E)\, (1 \pm e^{-\beta E}) = 0\ , \tag{2.9}$$

where the upper (lower) sign refers to the case where the two operators anticommute (commute). One can also easily establish a connexion between the spectral functions of the products, the commutator, and the anticommutator of two operators. Indeed, putting

$$\langle [C_1(x), C_2(x')]_{\pm} \rangle = \int_{-\infty}^{+\infty} dE\, e^{-iEt}\, J_{\pm}(\lambda, \lambda'; E)\ ,$$

we can use (2.6) and (2.7) to get

$$J_+(\lambda, \lambda'; E) = J_-(\lambda, \lambda'; E) \coth \tfrac{1}{2}\beta E = (1 + e^{-\beta E})\, J(\lambda, \lambda'; E)\ . \tag{2.10}$$

Finally, we see by comparing (2.6) and (2.7) that

$$K'(\lambda, \lambda'; t) = K(\lambda, \lambda'; t - i\beta)\ . \tag{2.11}$$

We shall obtain still a few more equations satisfied by the spectral function J. We shall put indices C_1 and C_2 on J to indicate the order in which the operators occur (to simplify our equations we have dropped the explicit mentioning of the variables λ and λ'):

$$\langle C_1(x) C_2(x') \rangle = \int_{-\infty}^{+\infty} dE\, e^{-iE(x_0 - x_0')}\, J_{C_1C_2}(E)\ .$$

Replacing now $C_1(x)$ and $C_2(x')$ by $C_2^+(x')$ and $C_1^+(x)$, respectively, we get

$$\langle C_2^+(x') C_1^+(x) \rangle = \int_{-\infty}^{+\infty} dE\, e^{-iE(x_0 - x_0')}\, J_{C_2^+C_1^+}(E)\ . \tag{2.12}$$

On the other hand, we can rewrite the right-hand side of (2.12) either as the complex conjugate of (2.6) or as the average of the rearranged product of $C_1^+(x)$ and $C_2^+(x')$ (see (2.7)):

$$\langle C_2^+(x') C_1^+(x) \rangle = \int_{-\infty}^{+\infty} dE\, e^{iE(x_0 - x_0')}\, J^+_{C_1C_2}(E) \tag{2.12a}$$

$$= \int_{-\infty}^{+\infty} dE\, e^{-iE(x_0 - x_0')}\, e^{-\beta E}\, J_{C_1^+C_2^+}(E)\ . \tag{2.12b}$$

By comparing the Fourier coefficients in (2.12) to (2.12b) we get for real E:

$$J^{+}_{C_1 C_2}(E) = J_{C_2^{+} C_1^{+}}(E) , \tag{2.13}$$

$$J^{+}_{C_1 C_2}(E) = J_{C_1^{+} C_2^{+}}(E)\, e^{-\beta E} , \tag{2.13a}$$

$$J_{C_2^{+} C_1^{+}}(-E) = J_{C_1^{+} C_2^{+}}(E)\, e^{-\beta E} . \tag{2.13b}$$

By putting $C_1 = C_2^{+}$ we see from (2.13) that $J_{C_1 C_1^{+}}$ is real:

$$J^{+}_{C_1 C_1^{+}}(E) = J_{C_1 C_1^{+}}(E) . \tag{2.14}$$

Let, moreover, the equations of motion be invariant under time-reversal, that is, under the transformation

$$x_0 \to - x_0 , \quad i \to - i . \tag{2.15}$$

Perform now in (2.6) the transformation

$$t \to - t , \quad i \to - i .$$

The left-hand side of (2.6) remains then unchanged while because of the interchange of i and - i on the right-hand side J is replaced by J^{+}:

$$K(x, x') = \langle C_1(x) C_2(x') \rangle = \int_{-\infty}^{+\infty} dE\; e^{-iEt}\, J^{+}_{C_1 C_2}(\lambda, \lambda'; E) . \tag{2.16}$$

Comparing (2.16) with (2.6) we see that in this case J is a real function:

$$J_{C_1 C_2}(\lambda, \lambda'; E) = J^{+}_{C_1 C_2}(\lambda, \lambda'; E) . \tag{2.17}$$

It follows from this that the following averages must also be real:

$$\langle C_1(\lambda, x_0) C_2(\lambda', x_0) \rangle = \int_{-\infty}^{+\infty} dE\, J_{C_1 C_2}(\lambda, \lambda'; E) . \tag{2.18}$$

Let, moreover, the operators C_1 and C_2 be Hermitean. We get from (2.6) and (2.7)

$$\langle [C_1(\lambda, x_0), C_2(\lambda', x_0)]_- \rangle = \int_{-\infty}^{+\infty} dE\, J_{C_1 C_2}(\lambda, \lambda'; E)\, (1 - e^{-\beta E}) .$$

If we now take the complex conjugate, we see that the left-hand side changes sign while the right-hand side remains unchanged because of (2.17). It follows thus that if C_1 and C_2 are Hermitean and if their equations of motion are invariant under time-reversal (2.15) we have

$$\int_{-\infty}^{+\infty} dE\, J(\lambda, \lambda'; E)\, (1 - e^{-\beta E}) = 0 . \tag{2.19}$$

The study of time correlations in the system is thus reduced to a study of the analytical properties of the spectral functions (2.5). In

particular, it is of great interest to find the delta-function-like singularities of $J(\lambda, \lambda'; E)$ on the real axis for the case $C_2 = C_1^+$ and $\lambda = \lambda'$. Indeed, let the corresponding singularities be E_i. It is clear that when they exist, the function $K(\lambda, \lambda'; t)$ oscillates with the frequencies * E_i. It is clear from expression (1.14) for the quantum-mechanical average (and also from the definition of the spectral function (2.5)) that the quantities E_i are at $T = 0$ the exact energy eigenvalues of the system. If the quantities E_i exist at all at $T \neq 0$, they depend on the temperature and on the chemical potential of the system and we can therefore not give an exact mechanical interpretation of them; it is, however, clear from (2.6) and (2.7) that they characterise undamped motions in the system. We are thus in a natural way led to a definition of the concept of a "temperature-dependent energy spectrum", which we mentioned in the introduction. It is clear from (2.5) that the values E_i are differences of the kind $E_n - E_{n'}$. This means, in particular, that at $T = 0$ they are the energies of the excitations in the system, calculated with respect to the ground state energy (which can simply be assumed to be equal to zero).

The use of the spectral functions enables us thus to determine directly the energy spectrum of the system.

To avoid misunderstandings we note the following facts. We can find at $T = 0$ such an operator C_1 (which will depend on n) that $C_1^+ \Phi_0 = \Phi_n$, so that the corresponding $J(\lambda, \lambda'; E)$ will have a delta-function-like singularity (this is simply the definition of the operator C_1^+). The determination of such operators is, however, equivalent to the exact solving of the Schrödinger equation for the given many-body system and is practically impossible to do (in cases which are of any interest). We can only state confidently that the simple combinations of the type $C_1 = a$ or $C_1 = a^+ a$, which we use in the following, will not have this property, and that thus the corresponding functions $K(x, x')$ will not oscillate, but be damped, as functions of the time. The singularities of the spectral functions $J(\lambda, \lambda'; E)$ have accordingly a more complicated character, and cannot be reduced simply to poles. The situation is more complicated at $T \neq 0$. Indeed, in that case we do not have a ground state average, but an average over a mixture. On the right hand side of (2.5) there will thus occur all possible matrix elements $(\Phi_n, C_1^+ \Phi_{n'})$ and the functions $K(x, x')$ can only in exceptional circumstances turn out to be oscillatory. This occurs, for instance, for the case of perfect Bose- or Fermi-gases (when there is no external field) when we take $C_1^+ = a^+(\vec{p}, s)$, where $a^+(\vec{p}, s)$ is the operator which creates a particle with a given momentum $\vec{p}$ and spin s. Indeed, the states of a perfect gas of freely moving particles are completely determined by given the occupation numbers $n(\vec{p}, s)$ of the "single-particle" states with given momenta

* The terms "frequency" and "energy difference" are used here and henceforth as synonyms because we have taken $\hbar = 1$.

and spins. The indices n and n' indicate the complete set of numbers $n(\vec{p},s)$, and the eigenfunctions Φ_n are products of δ-functions of the form

$$\Phi_{n'} = \prod_{\vec{p},s} \delta\,[n(\vec{p},s) - n_0(\vec{p},s)]\,,$$

where the n_0 are given numbers. It is clear that the operators a and a^+ change $\Phi_{n'}$ into another function of the same type, that is, the expressions $a\Phi_{n'}$ and $a^+\Phi_{n'}$ are also, whatever the value of n', eigenfunctions of H'. In the general case, however, there is always damping. The reason for this is that when there are interactions between the particles of a system with a continuous (or almost continuous) energy spectrum there is always exchange of energy, momentum, and so on, between different degrees of freedom. Mathematically the presence of damping shews itself in a displacement of the poles of the spectral functions from the real axis into the complex plane; there may appear singularities of a more complex nature on the real axis. Depending on the specific form of the operators C_1 and C_2 in (1.15), the poles which determine the damping must lie either in the upper or in the lower E-half-plane (see section 5).

The singularities of the spectral functions determine therefore only in exceptional cases truly stationary states of the system. However, if the damping is sufficiently small one can talk about quasi-stationary states. The corresponding quantities (1.15) are (for $t > 0$) of the form $e^{-i\omega t} f(t)$, there the (real) frequencies ω are connected with the singularities of the functions $J(\lambda, \lambda'; E)$, while the function $f(t)$ describes the damping ($f(t) \to 0$, as $|t| \to \infty$). The parameters determining the "rate of decrease" of $f(t)$ ("damping constants") must then be small compared to the frequencies ω reckoned from the ground state energy of the system (condition for quasi-stationary behaviour). Statistical mechanics usually deals with such quasi-stationary states (see the Introduction).

A study of the analytical properties of the spectral functions enables us in principle to determine the appropriate frequencies and damping constants, while guaranteeing an automatic check-up on the condition of quasi-stationarity. We shall in the following always mean these quasi-stationary states when we speak about the energy spectrum of the system (in particular, also when $T = 0$).

3. GREEN FUNCTIONS AND THEIR SPECTRAL REPRESENTATION *

When studying the structure of spectral functions of the kind (2.5) it is useful to be able to go into the complex E-plane. In that connexion it is advisable to introduce the functions

* See Bonch-Bruevich (1956b), Landau (1958a), Bogolyubov and Tyablikov (1959), Kogan (1959), and Bonch-Bruevich and Kogan (1960).

$$K_r(x,x') = i\,\langle C_1(x)C_2(x')\rangle\,\theta(t) \equiv \ll C_1(x)C_2(x')\gg_r , \tag{3.1}$$

$$K_r^{(\pm)}(x,x') = i\,\langle [C_1(x), C_2(x')]_\pm\rangle\,\theta(t) \equiv \ll C_1(x)\ C_2(x')\gg_r^{(\pm)} , \tag{3.2}$$

$$K_a(x,x') = -\,i\,\langle C_1(x)C_2(x')\rangle\,\theta(-t) \equiv \ll C_1(x)C_2(x')\gg_a , \tag{3.3}$$

$$K_a^{(\pm)}(x,x') = -\,i\,\langle [C_1(x), C_2(x')]_\pm\rangle\,\theta(-t) \equiv \ll C_1(x)\ C_2(x')\gg_a^{(\pm)} . \tag{3.4}$$

In these formulae, $\theta(t)$ is the well-known step function

$$\theta(t) = \begin{cases} 0 , & \text{if} \quad t < 0 , \\ 1 , & \text{if} \quad t > 0 . \end{cases}$$

The functions (3.1) to (3.4) have thus a singularity at $t = x - x' = 0$.

The expressions (3.1) and (3.2) are called retarded, and the expressions (3.3) and (3.4) advanced Green functions (hence the indices "r" and "a"). The reason for this nomenclature will become clear in section 7 where we obtain equations for some functions of the type (3.1) to (3.4) which are most often encountered.

We shall assume that the spectral function $J(\lambda, \lambda'; E)$ corresponding to $\langle C_1(x)C_2(x')\rangle$ decreases sufficiently rapidly as $E \to \infty$. Our calculations in sections 3 to 5 will all be made under this assumption. We note that the generalisation to the case where the spectral functions do not decrease as $E \to \infty$ can be made in exactly the same way as is done in field theory (Bogolyubov and Shirkov 1957).

In equilibrium the functions (3.1) to (3.4) depend only on the difference of the time arguments $x_0 - x_0' = t$. To simplify the equations, we introduce an index j which will stand for either "r" or "a", and we put

$$K_j(\lambda, \lambda'; t) = \int_{-\infty}^{+\infty} dE\ K_j(\lambda, \lambda'; E)\ e^{-iEt} , \tag{3.5}$$

$$K_j(\lambda, \lambda'; t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt\ K_j(\lambda, \lambda'; t)\ e^{iEt} . \tag{3.6}$$

From (3.1), (3.2), and (3.6) we see that the function $K_r(\lambda, \lambda'; E)$ is analytic in the upper half-plane of the complex variable E. Indeed, when $t < 0$, $K_r(\lambda, \lambda'; t) = 0$, while for $t > 0$ the exponential e^{iEt} contains a factor $e^{-t\,\mathrm{Im}E}$, which decreases exponentially when $\mathrm{Im}\ E > 0$, and thus ensures the convergence both of the integral in (3.6) and of all its derivatives with respect to E. Similarly, the function $K_a(\lambda, \lambda'; E)$ turns out to be analytic in the lower E-half-plane.

One can easily connect the Fourier transforms (3.6) of the Green functions (3.5) with the spectral functions $J(\lambda, \lambda'; E)$ introduced in the preceding section. Indeed, we get by using (2.1) to (2.5)

$$K_r(\lambda, \lambda'; t) = i\ \theta(t) \int_{-\infty}^{+\infty} dE\ e^{-iEt} J(\lambda, \lambda'; E) ;$$

comparing this with (3.5) we get (for real E)

$$K_r(\lambda, \lambda'; E) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dE' \frac{J(\lambda, \lambda'; E')}{E' - E - i\varepsilon}, \tag{3.7}$$

where ε is a positive quantity. Here and henceforth we shall always assume that in analytic expressions we bear in mind the limit as $\varepsilon \to 0$ *.

Similarly we have

$$K_a(\lambda, \lambda'; E) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dE' \frac{J(\lambda, \lambda'; E')}{E' - E + i\varepsilon}. \tag{3.8}$$

We have thus in the complex E-plane

$$\frac{1}{2\pi i} \int_{-\infty}^{+\infty} dE' \frac{iJ(\lambda, \lambda'; E')}{E' - E} = \begin{cases} K_r(\lambda, \lambda'; E), & \operatorname{Im} E > 0, \\ K_a(\lambda, \lambda'; E), & \operatorname{Im} E < 0. \end{cases} \tag{3.9}$$

The left hand side of (3.9) is a Cauchy-type integral. Indeed, K_r and K_a together can be considered to be one analytical function $K(\lambda, \lambda'; E)$ defined in the whole of the complex E-plane with, generally speaking, a cut along the real axis. It is also clear that one can directly express the spectral function $J(\lambda, \lambda'; E)$ in terms of the limiting values of $K(\lambda, \lambda'; E)$ at the upper and lower edges of the cut. Indeed, when we approach the real axis from above and from below we get for the corresponding limiting values of (3.9) **

$$\begin{aligned} -iK(\lambda, \lambda'; E+i\varepsilon) &= \tfrac{1}{2} J(\lambda, \lambda'; E) + \frac{1}{2\pi i} \int_{-\infty}^{+\infty} dE' \, \mathcal{P} \frac{J(\lambda, \lambda'; E')}{E' - E}, \\ -iK(\lambda, \lambda'; E-i\varepsilon) &= -\tfrac{1}{2} J(\lambda, \lambda'; E) + \frac{1}{2\pi i} \int_{-\infty}^{+\infty} dE' \, \mathcal{P} \frac{J(\lambda, \lambda'; E')}{E' - E}, \end{aligned} \tag{3.10}$$

from which it follows that

$$\begin{aligned} J(\lambda, \lambda'; E) &= -i \{K(\lambda, \lambda'; E+i\varepsilon) - K(\lambda, \lambda'; E-i\varepsilon)\} \\ &\equiv -i \{K_r(\lambda, \lambda'; E) - K_a(\lambda, \lambda'; E)\}. \end{aligned} \tag{3.11}$$

We note that we have not made any assumptions about whether the spectral function is real.

Similar spectral representations also occur for the functions $K_j^{(\pm)}$. We get, for instance, by using (2.2) to (2.4)

* (Note by the translator) One obtains (3.7) by putting $\theta(t) = 0$, if $t < 0$; $\theta(t) = e^{-\varepsilon t}$ $(\varepsilon \to +0)$, if $t > 0$.

** One can use equations (3.7) and (3.8) and the identity (x real) $1/(x + i\varepsilon) = \mathcal{P}(1/x) + \pi i \delta(x)$, where $\mathcal{P}$ indicates that the principal value must be taken of any integral where this symbol occurs.

$$K_r^{(\pm)}(x,x')$$

$$= i\theta(t) \sum_{n,n'} p_n \{(\Phi_n, C_1(\lambda, x_0=0)\Phi_{n'})(\Phi_{n'}, C_2(\lambda', x_0=0)\Phi_n)\, e^{-i(E_{n'}-E_n)t}$$

$$\pm (\Phi_n, C_2(\lambda', x_0=0)\Phi_{n'})(\Phi_{n'}, C_1(\lambda, x_0=0)\Phi_n)\, e^{-i(E_n-E_{n'})t}\} . \qquad (3.12)$$

If we interchange the summation indices n and n' in the second term within the braces and use (2.1) and (2.5) we find finally

$$K_j^{(\pm)}(\lambda, \lambda'; t) = \int_{-\infty}^{+\infty} dE\, K_j^{(\pm)}(\lambda, \lambda'; E)\, e^{-iEt} , \qquad (3.13)$$

where

$$K_r^{(\pm)}(\lambda, \lambda'; E) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dE' \, \frac{J(\lambda, \lambda'; E')}{E' - E - i\varepsilon} (1 \pm e^{-\beta E'}) , \qquad (3.14)$$

$$K_a^{(\pm)}(\lambda, \lambda'; E) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dE' \, \frac{J(\lambda, \lambda'; E)}{E' - E + i\varepsilon} (1 \pm e^{-\beta E'}) . \qquad (3.15)$$

We see again that $K_a^{(\pm)}(\lambda, \lambda'; E)$ and $K_r^{(\pm)}(\lambda, \lambda'; E)$ (or $K_a^{(-)}$ and $K_r^{(-)}$) together can be considered to be one analytical function $K^{(\pm)}$ of the complex variable E (with a cut along the real axis). For the spectral function we get easily a formula similar to (3.11):

$$J(\lambda, \lambda'; E) = \frac{-i}{1 \pm e^{-\beta E}} [K^{(\pm)}(\lambda, \lambda'; E+i\varepsilon) - K^{(\pm)}(\lambda, \lambda'; E-i\varepsilon)] ; \qquad (3.16)$$

E is here real.

We saw in section 2 that both the ordinary ensemble averages and the time-correlation functions of two arbitrary dynamical variables can be expressed directly in terms of the appropriate spectral function J (see (2.6) to (2.9)). The problem of evaluating these functions is thus reduced to finding the Fourier transforms of the corresponding Green functions. This method turns out to be in a number of cases much more convenient than a direct solution of the chain of equations for the successive operators $\rho_1, \rho_2, \ldots$

We finally introduce the so-called "causal" Green function *:

$$K_c(x, x') = i \langle T[C_1(x) C_2(x')] \rangle . \qquad (3.17)$$

The symbol T denotes here the time-ordering of a product of operators:

$$T[C_1(x)C_2(x')] = \begin{cases} C_1(x)C_2(x') , & x_0 > x_0' , \\ \eta C_2(x')C_1(x) , & x_0 < x_0' . \end{cases} \qquad (3.18)$$

The quantity η is equal to + 1 or - 1 depending on the parity of the permutation of the fermion creation and annihilation operators if one

* We discuss in appendix I the reason for calling this Green function "causal" and its role in quantum field theory.

changes from C_1C_2 to C_2C_1. If C_1 and C_2 contain only boson operators, $\eta = +1$. It is, in particular, clear from the definition that one may assume that all boson operators are commuting behind the T-sign, and that all fermion operators anticommute. It is clear that the function $K_c(x, x')$ is a linear combination of K_r and K_a (with a different order of the operators). In the same way as we obtained (3.12) to (3.15), we get easily

$$K_c(\lambda, \lambda'; t) = \int_{-\infty}^{+\infty} dE\, K_c(\lambda, \lambda'; E)\, e^{-iEt}\,, \tag{3.19}$$

$$K_c(\lambda, \lambda'; E) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dE' \left[\frac{J(\lambda, \lambda'; E')}{E' - E - i\varepsilon} - \eta \frac{J(\lambda, \lambda'; E')\, e^{-\beta E'}}{E' - E + i\varepsilon}\right]. \tag{3.20}$$

From (2.11) we see that the causal Green function satisfies the relation

$$K_c(t)\,|_{t>0} = \eta\, K_c(t+i\beta)\,|_{t<0}\,. \tag{3.21}$$

It follows from (3.20) that, in contradistinction to K_j and $K_j^{(+)}$, the function $K_c(\lambda, \lambda'; E)$ is, generally speaking, not an analytical function, and can not be continued into the complex plane. It is, however, important that the same spectral function $J(\lambda, \lambda'; E)$ occurs in all Green functions K_j, $K_j^{(+)}$, and K_c for given operators C_1 and C_2. It is therefore immaterial which of the Green functions we use, if we wish to study the energy spectrum and the matrix elements of the operators ρ_S.

We shall now establish some symmetry properties of Green functions.

We shall slightly rewrite (3.2) and (3.3)

$$\ll C_1(x)\,|\,C_2(x')\gg_r^{\pm} = i\,\theta(x_0 - x_0')\,\langle C_1(x)C_2(x') \pm C_2(x')C_1(x)\rangle\,; \tag{3.22}$$

$$\ll C_1(x)\,|\,C_2(x')\gg_a^{\pm} = i\,\theta(x_0' - x_0)\,\langle C_1(x)C_2(x') \pm C_2(x')C_1(x)\rangle\,; \tag{3.23}$$

$$\ll C_1(x)\,|\,C_2(x')\gg_c = i\langle T\{C_1(x)C_2(x')\}\rangle$$

$$= i\langle \theta(x_0 - x_0')C_1(x)C_2(x') + \eta\theta(x_0' - x_0)C_2(x')C_1(x)\rangle\,. \tag{3.24}$$

From (3.22) to (3.24) it follows that

$$\ll C_2(x')\,|\,C_1(x)\gg_a^{\pm} = \mp \ll C_1(x)\,|\,C_2(x')\gg_r^{\pm}\,; \tag{3.25}$$

$$\ll C_2(x')\,|\,C_1(x)\gg_c = \eta \ll C_1(x)\,|\,C_2(x')\gg_c\,. \tag{3.26}$$

Using (3.13) to (3.15), (3.19), and (3.20) to perform a Fourier transformation we get for real E:

$$K_{a,C_2C_1}^{\pm}(E) = \mp K_{r,C_1C_2}(-E)\,; \tag{3.27}$$

$$K_{c,C_2C_1}(E) = \eta\, K_{c,C_1C_2}(-E)\,. \tag{3.28}$$

Let us continue (3.27) into the complex E-plane. Using (3.14) and (3.15) we see that the functions $K^{\pm}_{r,C_1C_2}(-E)$ and $E^{\pm}_{a,C_2C_1}(E)$ are analytical in the same part of the E-plane. Since these functions are the limiting values of the functions $K^{\pm}_{C_1C_2}(-E)$ and $K^{\pm}_{C_2C_1}(E)$ (see (3.14) and (3.15)) we have in the complex plane:

$$K^{\pm}_{C_2C_1}(E) = \mp K^{\pm}_{C_1C_2}(-E) . \tag{3.29}$$

We see, moreover, from (3.22) and (3.23) that

$$[\ll C_1(x) | C_2(x') \gg^{\pm}_j]^+ = \mp \ll C_1^+(x) | C_2^+(x') \gg^{\pm}_j . \tag{3.30}$$

We shall now use (3.14) and (3.15) to change to the Fourier transforms of the Green functions. By comparing the Fourier coefficients we see easily that on the real axis we have

$$[K^{\pm}_{j,C_1C_2}(E)]^+ = + K^{\pm}_{j,C_1C_2}(-E) . \tag{3.31}$$

Let, moreover, the Heisenberg equations of motion be invariant under the transformation

$$t \to -t , \quad i \to -i . \tag{3.32}$$

As the spectral functions are real (see (2.17)) we get then

$$\langle C_1(x)C_2(x') \rangle = \langle C_2^+(x)C_1^+(x') \rangle , \quad \langle C_2(x')C_1(x) \rangle = \langle C_1^+(x')C_2^+(x) \rangle . \tag{3.33}$$

From this we get

$$\ll C_1(x) | C_2(x') \gg_j = \ll C_2^+(x) | C_1^+(x') \gg_j , \tag{3.34}$$

$$\ll C_1(x) | C_2(x') \gg^{\pm}_j = \ll C_2^+(x) | C_1^+(x') \gg^{\pm}_j , \tag{3.35}$$

and finally for the Fourier transform for real E

$$K_{j,C_1C_2}(\lambda, \lambda'; E) = K_{j,C_2^+C_1^+}(\lambda, \lambda'; E) , \tag{3.36}$$

$$K^{\pm}_{j,C_1C_2}(\lambda, \lambda'; E) = K^{\pm}_{j,C_2^+C_1^+}(\lambda, \lambda'; E) . \tag{3.37}$$

In conclusion we must make two more remarks. First of all, it is clear from (3.1) to (3.4) and (3.17) that all Green functions considered by us are uniquely defined, only if $x_0' \neq x_0$. If the time-arguments are the same, they have singularities and these lead ultimately to the appearance of the denominators $E - E' + i\varepsilon$. This fact leads us to writing K_r, K_a, and so on, as a Cauchy integral, that is, it enables us to consider the Green function in the whole of the complex plane, but it also leads to the necessity to state specifically which limiting value we have in mind as $x_0' \to x_0$ (compare section 5). Secondly, we restricted ourselves in this section to double-time quantities only, since they are sufficient to solve the specific problems which we consider in this book. It is, however, possible to ob-

tain spectral representations also for multiple-time Green functions (see appendix IV).

4. THE DIAGONAL ELEMENTS OF THE GREEN FUNCTIONS; DISPERSION RELATIONS *

In this section we consider the important case where $C_2 = C_1^+$ and $\lambda' = \lambda$. We are thus interested in quantities such as

$$K_r(\lambda, t) = i\theta(t) \langle C_1(\lambda, x_0) C_1^+(\lambda, x_0') \rangle . \tag{4.1}$$

The functions K_a, $K_a^{(+)}$, $K_r^{(+)}$, K_c are similarly defined. They define the diagonal matrix elements of the operators ρ_1, ρ_2, ...; we shall consider them also when we study the energy spectrum of the system (section 2). In the case of a continuous spectrum it is possible that, for instance, $K_r(\lambda, \lambda'; E) \sim \delta(\lambda - \lambda')$. (This occurs, for instance, for a spatially homogeneous system if the λ are the momentum components.) In such a case we must understand by the diagonal elements which occur in the following relations the coefficients in front of the δ-functions.

By virtue of (2.5) we have now

$$\begin{aligned} J(\lambda, \lambda; E) \equiv J(\lambda, E) &= \sum_{n,n'} p_n (\Phi_n, C\ (\lambda, x_0=0) \Phi_{n'}) (\Phi_{n'}, C_1^+(\lambda, x_0'=0) \Phi_n) \delta(E - E_{n'} + E_n) \\ &= \sum_{n,n'} p_n\ \delta(E - E_{n'} + E_n)\ |(\Phi_n, C_1 \Phi_{n'})|^2 \geq 0 . \end{aligned} \tag{4.2}$$

The spectral function is thus a real, positive quantity. Equation (3.11) gives then for real E

$$J(\lambda, E) = \operatorname{Im} K_r(\lambda, E) - \operatorname{Im} K_a(\lambda, E) . \tag{4.3}$$

The study of the energy spectrum of the system is thus reduced to a study of the singularities of the imaginary part of the analytical function $K(\lambda, E)$ of the complex variable E. Moreover, if we separate in (3.7) and (3.8) the real and the imaginary parts, we get by virtue of (3.11)

$$J(\lambda, E) = 2 \operatorname{Im} K_r(\lambda, E) = -2 \operatorname{Im} K_a(\lambda, E) , \tag{4.4}$$

$$\operatorname{Re} K_j(\lambda, E) = \pm \frac{1}{\pi} \int_{-\infty}^{+\infty} dE'\ \mathcal{P}\ \frac{\operatorname{Im} K_j(\lambda, E')}{E' - E} . \tag{4.5}$$

The plus-sign refers here to $j = r$, and the minus- sign to $j = a$. One obtains similar relations for the other Green functions:

* See Bonch-Bruevich (1956b), Landau (1958a), Bogolyubov and Tyablikov (1959), Kogan (1959), and Bonch-Bruevich and Kogan (1960).

$$J(\lambda, E) = \frac{2 \operatorname{Im} K_r^{(\pm)}(\lambda, E)}{1 \pm e^{-\beta E}} = -\frac{2 \operatorname{Im} K_a^{(\pm)}(\lambda, E)}{1 \pm e^{-\beta E}}, \tag{4.6}$$

$$\operatorname{Re} K_r^{(\pm)}(\lambda, E) = \frac{1}{\pi} \int_{-\infty}^{+\infty} dE' \, \mathcal{P} \frac{\operatorname{Im} K_r^{(\pm)}(\lambda, E')}{E' - E}, \tag{4.7}$$

$$\operatorname{Re} K_a^{(\pm)}(\lambda, E) = -\frac{1}{\pi} \int_{-\infty}^{+\infty} dE' \, \mathcal{P} \frac{\operatorname{Im} K_a^{(\pm)}(\lambda, E')}{E' - E}, \tag{4.8}$$

$$J(\lambda, E) = \frac{2 \operatorname{Im} K_c(\lambda, E)}{1 + \eta e^{\beta E}}, \tag{4.9}$$

$$\operatorname{Re} K_c(\lambda, E) = \frac{1}{\pi} \int_{-\infty}^{+\infty} dE' \frac{1 - \eta e^{-\beta E'}}{1 + \eta e^{-\beta E'}} \mathcal{P} \frac{\operatorname{Im} K_c(\lambda, E')}{E' - E}. \tag{4.10}$$

In all formulae (4.4) to (4.10) E is a real quantity. The character of the singularities of the Green functions on the real axis are especially clear from (4.4) and (4.6): generally speaking, the imaginary part of $K(\lambda, E)$ has there a finite jump. An exception is the case where $J(\lambda, E)$ has a delta-function singularity when Im $K(\lambda, E)$ is different from zero only in separate points E_i. (We saw in section 2 that these points are at $T = 0$ the exact energy eigenvalues of the system.) Since the spectral function $J(\lambda, E)$ is non-negative according to (4.2), equations (4.6) and (4.9) determine also the sign of the imaginary parts of the corresponding Green functions. We draw attention to the essential difference in the behaviour of Im $K_{r,a}^{(+)}$ and Im K_c depending on whether there is a +-sign or a - -sign in the denominator in (4.6) and (4.9). When there is a plus-sign these functions have always the same sign (Im $K_r^{(+)} > 0$, Im $K_a^{(+)} < 0$, Im $K_c > 0$), but if there is a minus-sign they change sign in the point $E = 0$. We shall use this circumstance in the following to determine the chemical potential of a system (see section 5). We note also that in the case of a minus-sign in the denominators of (4.6) and (4.9) there can appear terms $C\delta(E)$ on the right-hand side of these equations. The magnitude of C is determined from additional considerations such as the condition that the number of particles be conserved.

One calls equations such as (4.5), (4.7), (4.8), or (4.10) dispersion relations. They are widely employed in modern quantum field theory (Bogolyubov, Medvedev, and Polivanov 1958). For our purposes it is important that it follows from these relations that once we know the imaginary part of one of the functions $K_r(\lambda, E)$, $K_a(\lambda, E)$, ... they are all completely determined. This is also true of the function $K(x, x')$ (when $\lambda' = \lambda$ and $C_2 = C_1^+$) which was introduced in section 2 and which is of immediate physical interest. We get, for instance, from (2.7), (4.4), (4.6), and (4.9)

$$\langle C_1^+(\lambda, x_0) C_1(\lambda, x_0') \rangle = 2 \int_{-\infty}^{+\infty} dE \frac{\operatorname{Im} K_c(\lambda, E)}{e^{\beta E} + \eta} e^{-iE(x_0 - x_0')}$$

$$= 2 \int_{-\infty}^{+\infty} dE \frac{\operatorname{Im} K_r^{(\pm)}(\lambda, E)}{e^{\beta E} \pm 1} e^{-iE(x_0 - x_0')} \quad (4.11)$$

When $x_0' = x_0$ these formulae express the diagonal matrix elements of the operators $\rho_1, \rho_2, \ldots$ in terms of the imaginary parts of the appropriate Green functions; when $x_0' \neq x_0$ they give the time-correlation functions.

The diagonal elements of the retarded and advanced Green functions satisfy an important inequality. Using (5.5), (3.6), and (2.5) we have for the Fourier transforms with respect to the time

$$\ll C_1(\lambda_1) | C_1(\lambda_1) \gg_j |_{E=0} = \frac{1}{2\pi} \sum_{n,n'} p_n \frac{|(\Phi_n, C_1(\lambda_1, x_0=0) \Phi_{n'})|^2}{E_{n'} - E_n \pm i\varepsilon}, \quad (4.12)$$

$$\ll C_2(\lambda_2) | C_2(\lambda_2) \gg_j |_{E=0} = \frac{1}{2\pi} \sum_{n,n'} p_n \frac{|(\Phi_n, C_2(\lambda_2, x_0'=0) \Phi_{n'})|^2}{E_{n'} - E_n \pm i\varepsilon}, \quad (4.13)$$

$$\ll C_1(\lambda_1) | C_2(\lambda_2) \gg_j |_{E=0}$$

$$= \frac{1}{2\pi} \sum_{n,n'} p_n \frac{(\Phi_n, C_1(\lambda_1, x_0=0) \Phi_{n'})(\Phi_{n'}, C_2(\lambda_2, x_0'=0) \Phi_n)}{E_{n'} - E_n \pm i\varepsilon}. \quad (4.14)$$

Here, as before, the plus-sign refers to $j = a$, and the minus-sign to $j = r$.

Multiplying the absolute magnitudes of (4.12) and (4.13), comparing this result with (4.14), and using the Schwartz inequality, we get

$$|\ll C_1(\lambda_1) | C_1(\lambda_1) \gg |_{E=0} |\ll C_2(\lambda_2) | C_2(\lambda_2) \gg |_{E=0}$$

$$\geq |\ll C_1(\lambda_1) | C_2(\lambda_2) \gg|^2_{E=0}. \quad (4.15)$$

This is the inequality mentioned above *.

5. THE SIMPLEST GREEN FUNCTIONS

We have up to now not made any special assumptions about the operators C_1 and C_2. We shall now consider special cases which will be of most interest in the following.

a. *The single-fermion Green function.* We put $C_1 = a$ and $C_2 = a^+$, where a^+ and a are the operators which create and annihilate fermions.

* The authors express their gratitude to N. N. Bogolyubov for drawing their attention to this inequality and the way to prove it.

The matrix elements occurring in (2.5) are then

$$(\Phi_n, a(\lambda)\Phi_{n'}) \qquad \text{and} \qquad (\Phi_n, a^+(\lambda)\Phi_{n'}) \,. \tag{5.1}$$

It is well known that they are non-vanishing, if the number of particles in the states n and n' differ by unity. It follows from this that the delta-function-like singularities of the spectral function in this case will determine the change in energy of the fermion-system when the number of particles in it is changed by unity. It is assumed here that the extra particle goes into the state λ (or is taken from it). We emphasise that we introduced the states λ in section 1 simply as some basis system which could be used to introduce second quantisation. There is, generally speaking, no reason whatever that they are stationary states; accordingly, the spectral function may well not have singularities of this kind. If there are no interparticle interactions, one can, however, always choose for the basis system the eigenfunctions of the Hamiltonian; $J(\lambda, E)$ has then delta-function-like singularities only in the points E which are simply the energy values of separate particles. When there are interactions, the states $a^+(\lambda)\Phi_n$ are, strictly speaking, always non-stationary. Accordingly, the singularities of the spectral function $J(\lambda, E)$ do not have a purely delta-function-like character, and the states $a^+(\lambda)\Phi_n$ are damped as $t \to \infty$ (see section 2). If the damping is sufficiently small, however, we can in accordance with our discussion in section 2 speak about quasi-stationary "single-particle" states which are characterised by an energy and damping. Indeed, if we evaluate the transition probabilities in a system under the influence of a harmonically oscillating external field, we check easily that the frequency which determines the oscillations of the amplitude of a state as $t \to \infty$ occurs in the energy conservation law (see the example in chapter VII). In that case, as always in such cases, the energy of a "single-particle" state is conserved only within a margin connected with the damping. We emphasise that in practical cases, the "single-particle" states refer not to separate particles, but to the system as a whole. In quantum field theory language this fact explains the term "dressed" particles (fermions). We easily see, by using (1.15) with $C_1 = a$ and $C_2 = a^+$, that the damping of fermion states is determined by the poles of the analytical continuation of the spectral function into the lower E-half-plane (when Re $E > 0$). The poles in the upper half-plane (when Re $E < 0$) describe the damping of the corresponding "hole" states. These poles are just the poles of the Green function $G_j(E)$ itself on an "unphysical" sheet which differs from the one defined by (3.14) and (3.15).

The corresponding Green functions are called single-fermion Green functions; we shall denote them by G:

$$G_C(x, x') = i\,\langle T[a(x)a^+(x')]\rangle, \; G_j^{(\pm)}(x,x') = \ll a(x)\,|a^+(x')\gg_j^{(\pm)} \,. \tag{5.2}$$

It is clear that (4.11) with $C_1 = a$ and $x_0 = x_0'$ leads to the distribution function $f(\lambda)$ (we bear in mind that here $\eta = -1$).

We note, in particular, two cases:

1) $\lambda = \{\vec{x}, s\}$: the position coordinates $\vec{x}$ and the spin variable s. The left-hand side of (4.11) is then for $x_0' = x_0$ the average concentration of electrons at $\vec{x}$ with spin s, and the total electron concentration $n(\vec{x})$ is given by the equations

$$n(\vec{x}) = 2\int_{-\infty}^{+\infty} dE\, \frac{\sum_s \operatorname{Im} G_c(\vec{x},s;E)}{e^{\beta E} - 1} = 2\int_{-\infty}^{+\infty} dE\, \frac{\sum_s \operatorname{Im} G_r^{(\pm)}(\vec{x},s;E)}{e^{\beta E} \pm 1} . \tag{5.3}$$

We emphasise here that one must put a minus-sign in the first denominator in (5.3) (and not a plus-sign, as one might have expected). We must draw attention to the fact that $n(\vec{x})$ can according to (5.2) also be written as

$$n(\vec{x}) = i \lim_{\substack{x' \to x \\ x_0' > x_0}} \sum_s G_c(x,s;x's) \equiv i \lim_{\substack{x' \to x \\ x_0' > x_0}} \operatorname{Tr} G_c(x,x') . \tag{5.4}$$

This equation determines how one must take the limit $x_0' \to x_0$ for the function $G_c(x,x')$ (compare the discussion at the end of section 2); we have thus

$$G_c(\lambda,x_0;\lambda',x_0) = \lim_{\substack{x_0' \to x_0 \\ x_0' > x_0}} G_c(\lambda,x_0;\lambda',x_0') . \tag{5.5}$$

2. $\lambda = \{\vec{p}, s\}$: the momentum $\vec{p}$ and the spin variable s. We shall now consider the case of a spatially uniform system when the function $G_c(\lambda,\lambda';t)$ is diagonal in the momentum; let it, moreover, also be diagonal in the spin. We go over to the momentum representation using the equation

$$G_c(\vec{x},x_0;\vec{x}',x_0) = \int d^4p\, G_c(\vec{p},p_0)\, e^{-i(px-px')} , \tag{5.6}$$

where $px = p_0x_0 - (\vec{p}\,.\,\vec{x})$, $d^4p = d^3\vec{p}\, dp_0$; we use here the variable p_0 instead of E for the sake of symmetry. Equation (4.11) (with $x_0' = x_0$) becomes now the general expression for the electron momentum distribution function $f(\vec{p})$. Using the normalisation implied in (5.6) we get

$$f(\vec{p}) = 2(2\pi)^3 \int_{-\infty}^{+\infty} dp_0\, \frac{\operatorname{Im} G_c(\vec{p},p_0)}{e^{\beta p_0} - 1} = 2(2\pi)^3 \int_{-\infty}^{+\infty} dp_0\, \frac{\operatorname{Im} G_r^{(\pm)}(\vec{p},p_0)}{e^{\beta p_0} \pm 1} \tag{5.7}$$

The function (5.7) is normalised to the occupation number.

We note that the following properties of the functions $G_j^{(+)}(\vec{p}, E)$ in the complex E-plane follow from the definition (3.29) *:

$$\ll a^+(\vec{p}) \mid a(\vec{p}) \gg_E = - \ll a(\vec{p}) \mid a^+(\vec{p}) \gg_{-E},$$

$$\ll a(-\vec{p}) \mid a(\vec{p}) \gg_E = - \ll a(\vec{p}) \mid a(-\vec{p}) \gg_{-E}, \qquad (5.8a)$$

$$\ll a^+(-\vec{p}) \mid a^+(\vec{p}) \gg_E = - \ll a^+(\vec{p}) \mid a^+(-\vec{p}) \gg_{-E}.$$

Moreover, it follows from the fact that the equations of motion (2.3) are invariant under time-reversal (if we change at the same time i to - i) and from (3.36) that

$$\ll a^+(-\vec{p}) \mid a^+(\vec{p}) \gg_E = \ll a(\vec{p}) \mid a(-\vec{p}) \gg_E . \qquad (5.8b)$$

Finally, it follows from the invariance with respect to spatial inversion that

$$\ll a(\vec{p}) \mid a(-\vec{p}) \gg_E = \ll a(-\vec{p}) \mid a(\vec{p}) \gg_E ,$$

$$\ll a^+(\vec{p}) \mid a^+(-\vec{p}) \gg_E = \ll a^+(-\vec{p}) \mid a^+(\vec{p}) \gg_E , \qquad (5.8c)$$

$$\ll a(\vec{p}) \mid a^+(\vec{p}) \gg_E = \ll a(-\vec{p}) \mid a^+(-\vec{p}) \gg_E .$$

We bear here in mind that the quantities E_n and $E_{n'}$ in (2.5) are by definition eigenvalues of the generalised Hamiltonian (1.7): $H' = H - \mu N$ (see section 1). Bearing in mind what we said in the foregoing about the matrix elements (5.1), we see that in the present case

$$E = W - \mu ,$$

where W is the difference between the eigenvalues of H belonging to states which differ by unity in the number of particles. (This equation is valid, because in the case considered here the operators H and N commute.) It follows, on the other hand, from (4.9) that in the present case (with a minus-sign in the denominator) the function Im $G_c(\lambda, E)$ changes sign together with E (we have sign Im $G_c(\lambda, E)$ = sign E so that there are no other points where the sign of the imaginary part of $G_c(\lambda, E)$ changes). We can thus formulate a rule to determine the chemical potential of a system of interacting fermions: the chemical potential μ is equal to the energy W where the imaginary part of the single-particle Green function, Im $G_c(\lambda, W-\mu)$, changes sign. (Instead of Im G_c we can also take Im $G_r^{(-)}(\lambda, E)$ or Im $G_a^{(-)}(\lambda, E)$.)

We shall consider especially the case of a perfect gas, that is a system of fermions moving in a given, constant external field, but without interparticle interactions (an analysis of this case is not only

* The authors are grateful to N. N. Bogolyubov for drawing their attention to the importance of these relations.

of interest methodically, but it also turns out to be useful for approximating the solutions of the equations for the complete Green functions (see section 11)). It is convenient to choose here for the parameters λ the quantum numbers characterising the stationary states of the separate particles in the given field. The corresponding energy eigenvalues and eigenfunctions (in the coordinate representation) will be denoted by $E(\lambda) = W(\lambda) - \mu$ and $\varphi_\lambda(\vec{x})$. The indices n and n' characterising the states of the whole system indicate in this case which of the single-particle states φ_λ are occupied; the total energy E_n is a sum of the energies of the separate particles in the occupied states.

One can easily evaluate here all the Green functions (which we give in this case a superscript "o"). Take, for instance, the causal function $G_c(\lambda, x_0; \lambda', x_0')$. From (3.17) and (3.18) we get

$$G_c(\lambda, x_0; \lambda', x_0') = i \langle T[a(\lambda, x_0)\, a^+(\lambda', x_0')] \rangle$$

$$= \begin{cases} i \langle a(\lambda, x_0) a^+(\lambda', x_0') \rangle , & x_0 > x_0' , \\ - i \langle a^+(\lambda', x_0') a(\lambda, x_0) \rangle , & x_0 < x_0' . \end{cases}$$

The time dependence of the operator $a(\lambda, x_0)$ is expressed in this case simply by the factor $\exp[-iE(\lambda)x_0]$; hence

$$\langle a^+(\lambda', x_0') a(\lambda, x_0) \rangle = \langle a^+(\lambda', 0) a(\lambda, 0) \rangle\, e^{-iE(\lambda)x_0 + iE(\lambda')x_0'} .$$

In the case considered different values of λ correspond to different eigenfunctions of the system; therefore

$$\langle a^+(\lambda', 0) a(\lambda, 0) \rangle = \delta(\lambda - \lambda') \langle a^+(\lambda, 0) a(\lambda, 0) \rangle = \delta(\lambda - \lambda')\, n_F(\lambda) , \qquad (5.9)$$

where $n_F(\lambda)$ is the average value of the occupation number of the state λ. It is clearly given by the usual Fermi-function (we remember that the latter is just obtained by evaluating the trace occurring in (5.9) (see, for instance, Bogolyubov 1949)). Similarly

$$\langle a(\lambda, x_0) a^+(\lambda', x_0') \rangle = e^{-iE(\lambda)x_0 + iE(\lambda')x_0'}\, \delta(\lambda - \lambda')\, [1 - n_F(\lambda)] . \qquad (5.10)$$

We have thus

$$G_c^{(o)}(\lambda, x_0; \lambda', x_0') = i\delta(\lambda - \lambda')\, e^{-iE(\lambda)(x_0 - x_0')} \{\theta(x_0 - x_0')\, [1 - n_F(\lambda)]$$

$$- \theta(x_0' - x_0)\, n_F(\lambda)\} , \qquad (5.11)$$

where

$$n_F(\lambda) = \frac{1}{e^{\beta W(\lambda) - \beta\mu} + 1} . \qquad (5.12)$$

For the Fourier transform we get

$$G_c^{(o)}(\lambda,\lambda';E) = -\frac{1}{2\pi}\,\delta(\lambda-\lambda')\left\{\frac{n_F(\lambda)}{E - E(\lambda) - i\varepsilon} + \frac{1 - n_F(\lambda)}{E - E(\lambda) + i\varepsilon}\right\}$$

$$\equiv \delta(\lambda-\lambda')\, G_c^{(o)}(\lambda,E)\ . \tag{5.13}$$

Accordingly we have in the coordinate representation (s and s' are spin coordinates)

$$G_c^{(o)}(\vec{x}, s, x_o; \vec{x}', s', x_o')$$

$$= \sum_\lambda \int_{-\infty}^{+\infty} dE\ \varphi_\lambda(\vec{x}, s)\ \varphi_\lambda^+(\vec{x}', s')\ e^{-iE(x_o - x_o')}\ G_c^{(o)}(\lambda, E) \tag{5.14}$$

(the sum over λ may, as always, also include an integral). The expression within the braces in (5.13) becomes discontinuous when there is complete degeneracy: as $T \to 0$, $n(\lambda) = 1$, if $W(\lambda) < \mu$, and $n(\lambda) = 0$, if $W(\lambda) > \mu$. It may be more convenient in that case to use the expression

$$G_c^{(o)}(\lambda, E) = -\frac{1}{2\pi}\,\frac{1}{E - E(\lambda) + i\varepsilon\ \mathrm{sign}\,[W(\lambda)-\mu]}\ , \tag{5.13a}$$

which is equivalent to (5.13) at $T = 0$.

Similarly, we get for the retarded and advanced Green functions

$$G_r^{(o)(+)}(\lambda,\lambda';E) = -\frac{1}{2\pi}\,\delta(\lambda-\lambda')\,\frac{1}{E - E(\lambda) + i\varepsilon}\ ,$$

$$G_a^{(o)(+)}(\lambda,\lambda';E) = -\frac{1}{2\pi}\,\delta(\lambda-\lambda')\,\frac{1}{E - E(\lambda) - i\varepsilon}\ , \tag{5.15}$$

$$G_r^{(o)}(\lambda,\lambda';E) = -\frac{1}{2\pi}\,\delta(\lambda-\lambda')\,\frac{1 - n_F}{E - E(\lambda) + i\varepsilon}\ ,$$

$$G_a^{(o)}(\lambda,\lambda';E) = -\frac{1}{2\pi}\,\delta(\lambda-\lambda')\,\frac{1 - n_F}{E - E(\lambda) - i\varepsilon}\ . \tag{5.16}$$

It is interesting to note that the "anticommutator" Green functions $G_J^{(o)(+)}$ for a free electron gas are in general temperature-independent.

It is clear that the poles of (5.13), (5.15), and (5.16) are, indeed, connected with the energy spectrum of the system. Using (4.3) (or (4.9)) with a minus-sign in the denominator) we can find the spectral function

$$J^{(o)}(\lambda, E) = [1 - n_F(\lambda)]\ \delta[E - E(\lambda)]\ . \tag{5.17}$$

As one should have expected, it turns out to behave like a delta-function. In the present case this result is trivial: there is no interaction between the particles, and there is therefore no damping, and the eigenvalues of the single-particle energy operator $W(\lambda)$ deter-

mine the exact changes in the energy of the whole system when the number of particles in the system changes by unity (when a particle in the state λ is added to the system, its total energy is increased by $G(\lambda)$).

By virtue of (5.13), the imaginary part of $G_c^{(o)}(\lambda, E)$ is

$$\operatorname{Im} G_c^{(o)}(\lambda, E) = \frac{1 - 2n_F(\lambda)}{2}\,\delta[E - E(\lambda)]$$

$$= \tfrac{1}{2}\tanh\left(\frac{\beta}{2}[W(\lambda) - \mu]\right)\delta[E - E(\lambda)]\,. \qquad (5.18)$$

It is clear that it changes sign at the point $W(\lambda) = \mu$, in accordance with the general results of section 4.

Using (5.18) we can easily verify also the validity of (4.11). In the present case it becomes an identity when $x_0' = x_0$.

We shall, finally, write down in explicit form the Green functions for the case of free particles moving in a cube of volume V when there is no external field. This case is of special interest for the following as we shall see in chapter IV that a whole number of problems in the electron theory of solids can be reduced to it. The role of λ is in this case played by the momentum $\vec{p}$ together with the spin quantum number σ.

We shall use as the boundary conditions at the surface of the cube the usual periodicity conditions (this is always done whenever we are not interested in surface effects as such). We have thus

$$\varphi_\lambda(\vec{x}) = V^{-\frac{1}{2}}\, S_\sigma(s)\, e^{i(\vec{p}\,.\,\vec{x})}\,,$$

where S is a spin function, and (5.14) gives

$$G_c^{(o)}(\vec{x}, s, x_0; \vec{x}', s', x_0')$$

$$= -\frac{\delta_{ss'}}{2\pi V}\sum_{\vec{p}}\int_{-\infty}^{+\infty} dE\; e^{-iE(x_0 - x_0')}\, e^{i(\vec{p}\,.\,\vec{x} - \vec{x}')}\left\{\frac{n_F(\vec{p})}{E - E(\vec{p}) - i\varepsilon} + \frac{1 - n_F(\vec{p})}{E - E(\vec{p}) + i\varepsilon}\right\}.$$

Changing here from a summation to an integration, replacing E by p_0 and using the normalisation (5.6), we get

$$G_c^{(o)}(\vec{x}, s, x_0; \vec{x}', s', x_0') = \delta_{ss'}\int d^4p\; e^{-i(px - px')}\, G_c^{(o)}(\vec{p}, p_0)\,, \qquad (5.19)$$

$$G_c^{(o)}(\vec{p}, p_0) = -\frac{1}{(2\pi)^4}\left\{\frac{n_F(\vec{p})}{p_0 - E(\vec{p}) - i\varepsilon} + \frac{1 - n_F(\vec{p})}{p_0 - E(\vec{p}) + i\varepsilon}\right\}$$

$$= -\frac{1}{(2\pi)^4}\cdot\frac{p_0 - E(\vec{p}) + i\varepsilon\,[2n_F(\vec{p}) - 1]}{[p_0 - E(\vec{p})]^2 + \varepsilon^2}\,. \qquad (5.20)$$

Similarly

$$G_r^{(o)}(\vec{p}, p_o) = -\frac{1}{(2\pi)^4} \cdot \frac{1 - n_F(\vec{p})}{p_o - E(\vec{p}) + i\varepsilon}$$
$$G_a^{(o)}(\vec{p}, p_o) = -\frac{1}{(2\pi)^4} \cdot \frac{1 - n_F(\vec{p})}{p_o - E(\vec{p}) - i\varepsilon}, \tag{5.21}$$

$$G_r^{(o)(+)}(\vec{p}, p_o) = -\frac{1}{(2\pi)^4} \cdot \frac{1}{p_o - E(\vec{p}) + i\varepsilon},$$
$$G^{(o)(+)}(\vec{p}, p_o) = -\frac{1}{(2\pi)^4} \cdot \frac{1}{p_o - E(\vec{p}) + i\varepsilon}. \tag{5.22}$$

As $T \to 0$ it is more convenient to use instead of (5.20) a formula which at $T = 0$ is equivalent to it (see the discussion of (5.13a)):

$$G_c(\vec{p}, p_o) = -\frac{1}{(2\pi)^4} \cdot \frac{1}{p_o - E(\vec{p}) + i\varepsilon \operatorname{sign}[W(\vec{p}) - \mu]}. \tag{5.23}$$

We draw attention to the close similarity between this expression and the causal single-fermion Feynman function, well-known from quantum field theory (Bogolyubov and Shirkov 1957). The vacuum of quantum field theory is here replaced by the ground state of the system of free particles (all levels with energies less than μ are occupied, while all levels with energies larger than μ are empty). We shall reckon the energies from μ. The function $G_c^{(o)}(x, x')$, and also the Feynman function, contains then only positive energies, if $x_o > x_o'$, and only negative energies, if $x_o' > x_o$. This property has sometimes been used as a boundary condition for choosing just the causal function from amongst all others (G_r, G_a, and so on). It is usually called the Feynman boundary condition. One should, however, note that the situation is only so simple in the case of free particles; if there are interparticle interactions the momentum distribution function is, generally speaking, different from the Fermi-function.

b. *The single-boson Green function.* We take again, as under a) $C_1 = a$, $C_2 = a^+$, but now the a^+ and a are the boson creation and annihilation operators. We shall denote them, as in the fermion case, by G. (Since the single-fermion and the single-boson Green functions can never be applied to the same particles, there can arise no misunderstanding.) The matrix elements occurring in the expansion (4.2) are, as before, of the kind (5.1). This enables us to interpret immediately the poles of the spectral function as the "dressed" boson spectrum. As under a) (4.11) gives us the distribution function of the particles with respect to λ; one must, however, bear in mind that now $\eta = +1$. Equations (5.3) remain thus valid; we need only change the sign in the denominators of the integrands oc-

curring in the expression containing Im G_c: instead of $e^{\beta E} - 1$ we now have $e^{\beta E} + 1$. We must also change the sign in (5.4): the particle density is now given by the formula

$$n(\vec{x}) = -i \lim_{\substack{x_0' \to x_0 \\ x_0' > x_0}} \mathrm{Tr}\, G_c(x, x') . \qquad (5.4a)$$

Like the single-fermion Green function, the single-boson Green function $G_\nu^{(-)}(\vec{p}, E)$ considered in the complex E-plane satisfies important relations of the kind (5.8a,b,c) which follow from the definition of $G_\nu^{(-)}$ and from the invariance properties of the equations of motion under time reversal and spatial inversion. The only difference is connected with the different commutator rules which hold for boson and fermion operators, and this leads to a change in sign of the right-hand sides of (5.8a).

c. *The double-time two-particle Green function.* We now put in (3.1) to (3.4) and (3.17):

$$C_1 = a^+(\vec{x}_1, x_0)a(\vec{x}_2, x_0) \quad \text{and} \quad C_2 = a^+(\vec{x}_1', x_0')a(\vec{x}_2', x_0') ,$$

where the a^+ and a are either fermion or boson operators. In other words, we shall consider functions of the type

$$G_{2,c} = i \langle T [a^+(\vec{x}_1, x_0)a(\vec{x}_2, x_0)a^+(\vec{x}_1', x_0')a(\vec{x}_2', x_0')] \rangle . \qquad (5.24)$$

It is clear that (5.24) is a particular case of a more general expression of the form

$$G_{2,c}(x_1, x_2, x_3, x_4) = i \langle T [a^+(x_1)a(x_2)a^+(x_3)a(x_4)] \rangle , \qquad (5.25)$$

which leads to (5.24) in the limit where the first two and the last two time arguments are equal. The quantity (5.25) is called the two-particle Green function (this term is connected with the fact that the operator occurring in (5.25), the average of which is taken, can change the state of two particles simultaneously).

The matrix elements occurring in the spectral function (4.2) corresponding to (5.24) are $(\Phi_n, a^+(x, 0)a(x', 0)\Phi_{n'})$. They are different from zero only if the number of particles in the states n and n' is the same. The poles of the spectral function determine now thus the excitation spectrum of a system with a given number of particles. One can easily evaluate functions such as (5.24) for the perfect gas. Let us, for instance, consider the retarded Green function for a completely degenerate Fermi-gas ($T = 0$) when there is no external field. Using (5.5) we get, when $x_0 \neq x_0'$

$$\begin{aligned} G_{2,r}(x, x') &= i n^2 + i G_r(x, x') G_r(x', x) \\ &= i n^2 + \frac{i}{(2\pi)^6} \int d^3\vec{p}\, d^3\vec{p}'\, \theta[W(\vec{p}) - \mu]\, \theta[\mu - W(\vec{p}')] \\ &\quad \times e^{i(\vec{p} - \vec{p}')\cdot(\vec{x} - \vec{x}') - i[W(\vec{p}) - W(\vec{p}')](x_0 - x_0')} , \end{aligned} \qquad (5.26)$$

where n is the constant particle concentration.

Using a formula such as (5.6) to introduce the Fourier transform $G_{2,r}(\vec{p},p_0)$, we see that the poles of Im $G_{2,r}(\vec{p},p_0)$ (that is, the poles of the spectral function) are

$$p_0 = W(\vec{p}) - W(\vec{p}') , \qquad W(\vec{p}) \geq \mu , \qquad W(\vec{p}') \leq \mu . \tag{5.27}$$

This is clearly the expression for the spectrum of excitations arising when electrons are kicked out of the Fermi sphere.

d. *The single-photon Green function.* We now put in (3.1) and the following equations $C_1 = A_\alpha(x)$, $C_2 = A_\beta(x')$, where A_α and A_β are the operators of the four-potential of the electromagnetic field, $\alpha = 0$, 1, 2, or 3. As was done by Bogolyubov and Shirkov (1957), it is convenient for us to choose the four components of the four-potential such that $\{A_1, A_2, A_3\} = \vec{A}$ is the vector potential, and $-A_0 = \varphi$ is the scalar potential. The electrical field strength and the magnetic field strength are thus given by the equations

$$E_i = \frac{\partial A_0}{\partial x_i} - \frac{1}{c_0}\frac{\partial A_i}{\partial x_0} \quad (i = 1,2, \text{ or } 3); \qquad \vec{B} = \operatorname{curl} \vec{A} = \mu \vec{H} .$$

Here c_0 is the velocity of light in vacuo. We shall characterise the optical properties of the medium (when there are no free charges) by scalar, real dielectric and magnetic susceptibilities ϵ and μ which we assume to be independent of position (we restrict ourselves thus to optically uniform and isotropic media far from an absorption band). The velocity of light in the medium we denote by $c = c_0/(\epsilon\mu)^{\frac{1}{2}}$.

We shall shew in appendix I that we can under these conditions completely eliminate ϵ and μ from the electrodynamical equations, if we introduce "renormalised" quantities

$$A_i^{(r)} = A_i , \qquad A_0^{(r)} = (\epsilon\mu)^{\frac{1}{2}} A_0 , \qquad e^{(r)} = (\tfrac{\mu}{\epsilon})^{\frac{1}{2}} e , \qquad W^{(r)} = \mu W$$

(e is the charge, and W any energy connected with the electromagnetic field, for instance, the energy of a free field or the energy of a charge in a field, and so on). The velocity of light c_0 is then everywhere replaced by c. In the following we shall (except in chapter VII) use only the renormalised quantities, and omit the superscript "r". The quantity λ is now the combination of the tensor index α and the position $\vec{x}$. The matrix elements occurring in (4.2) are

$$(\Phi_n, A_\alpha(\vec{x},x_0)\Phi_{n'}) . \tag{5.28}$$

They are non-vanishing if the number of photons in the states n and n' differs by unity, and the poles of the spectral function now determine thus the spectrum of "dressed" photons (that is, photons interacting with their surroundings). When we speak here about photons we have in mind not only the usual quanta of the transverse electromagnetic field, but also the longitudinal quanta (in a medium these can, in contradistinction to in vacuo, in fact be propagated).

One can easily see by using (1.15) that the damping of the photons is given by the poles of the analytical continuation of the spectral function in the lower half-plane (with Re $E > 0$). The corresponding Green function (with the opposite sign for the sake of convenience) is called the single-photon Green function; we shall denote it by D. Thus:

$$D_{c,\alpha\beta}(x,x') = -i\langle T[A_\alpha(x)A_\beta(x')]\rangle . \tag{5.29}$$

We shall use the same notation also for the phonon Green functions, bearing in mind that they will not be considered together with the photon Green functions. One could have called these functions single-boson functions, but we retain this term only for the "corpuscular" functions G to distinguish them from the "field" functions D. We note that in the framework of a non-relativistic theory the difference between these two kinds of functions is not just a semantic one: we shall see in the following that the G satisfy differential equations of the first order in time, while those for the D are of second order.

We shall be most interested in the spatially uniform case; we have then in accordance with (5.6)

$$D_{c,\alpha\beta}(x,x') = \int d^3\vec{k}\, d\omega\, e^{-i\omega(x_0-x_0')+i(\vec{k}.\vec{x}-\vec{x}')} D_{c,\alpha\beta}(\vec{k},\omega) . \tag{5.30}$$

It is clear that by virtue of the boson-character of the Hermitean operators $A_\alpha(x)$ we have (for real $\vec{k}$ and ω)

$$D_{c,\alpha\beta}(\vec{k},\omega) = D_{c,\alpha\beta}(-\vec{k},-\omega) . \tag{5.31}$$

If we use (5.31), we can write the dispersion relation (4.10) in a slightly more convenient form: we write the integral occurring in (4.10) as a sum of two integrals, taken, respectively from 0 to ∞, and from $-\infty$ to 0 and change in the second of these integrals the variable E' to $-E'$. If we remember that here $\eta = 1$, we find easily

$$\mathrm{Re}\, D_c(\vec{x},\vec{x}';E) = \frac{1}{\pi}\int_0^{+\infty} dE'^2\, \frac{1-e^{\beta E'}}{1+e^{\beta E'}}\, \mathcal{P}\, \frac{\mathrm{Im}\, D_c(\vec{x},\vec{x}';E')}{E'^2-E^2} . \tag{5.32}$$

We must notice that the function (5.29) is not uniquely defined, because of possible gauge transformations of the four-potential. Indeed, we can everywhere make the substitution

$$A_i(x) \to A_i(x) + \frac{\partial f}{\partial x_i} , \qquad A_0 \to A_0 + \frac{1}{c}\frac{\partial f}{\partial x_0} , \tag{5.33}$$

where f is an arbitrary twice differentiable scalar function.

For the sake of convenience we write

$$k_0 = \omega/c , \qquad k^2 = k_0^2 - \vec{k}^2 .$$

It is clear that under the transformation (5.33) the Fourier transform $D_{c,\alpha\beta}(\vec{k},\omega)$ is transformed according to the rule

$$D_{c,\alpha\beta}(\vec{k},\omega) \to D_{c,\alpha\beta}(\vec{k},\omega) + k_\alpha k_\beta F(k^2) , \qquad (5.34)$$

where $F(k^2)$ is connected with the Fourier transform of $f(x)$. Since all electrodynamic functions are gauge-invariant, $F(k^2)$ must not occur (and in fact does not occur (see Bogolyubov and Shirkov 1957)) in any observable quantities evaluated using (5.30). We can thus choose it in such a way that the function $D_{c,\alpha\beta}(\vec{k},\omega)$ has a more convenient form.

We note in this connexion that for an isotropic system the whole "tensor" part of $D_{c,\alpha\beta}(\vec{k},\omega)$ can be expressed simply in terms of the product $k_\alpha k_\beta$ and the unit tensor. We shall restrict ourselves in the following to this case. It is then convenient to put

$$D_{c,\alpha\beta}(\vec{k},\omega) = [g_{\alpha\beta} - (k_\alpha k_\beta/k^2)]\, D_c(\vec{k},\omega) , \qquad (5.35)$$

where

$$g_{\alpha\beta} = g^{\alpha\beta} = 0 , \quad \alpha \neq \beta ; \quad g_{oo} = -g_{11} = -g_{22} = -g_{33} = 1 . \qquad (5.36)$$

One can then easily verify that the function $D_{c,\alpha\beta}(x,x')$ satisfies a kind of "Lorentz condition":

$$\frac{1}{c}\frac{\partial D_{c,o\beta}(x,x')}{\partial x_o} - \frac{\partial D_{c,i\beta}(x,x')}{\partial x_i} = 0 . \qquad (5.37)$$

When verifying (5.37) one must bear in mind the well-known equality from electrodynamics (see Bogolyubov and Shirkov 1957 and (I.33))

$$<[A_\alpha(\vec{x},x_o), A_\beta(\vec{x}',x_o)]_-> = 0 .$$

We note that (5.37) is also valid for the functions $D^{(-)}_{r,a}$.

We shall see in chapter II that condition (5.37) ensures that the usual electrodynamical Lorentz condition is satisfied for the average (practically observed) potentials of the electromagnetic field which are evaluated taking the interaction with charged particles into account. This is the physical meaning of the choice (5.35).

The gauge-invariance of the theory enables us thus to reduce the tensor $D_{c,\alpha\beta}$ to only one scalar function, D_c.

In the general theory developed in the next two chapters we shall not explicitly specialise the form of the function $D_{c,\alpha\beta}$ (except when we consider the renormalisation group, when we shall use (5.35)). However, when we solve specific problems in chapters IV and V we use explicitly the gauge (5.35).

We consider finally, as under a), the particular case of a free electromagnetic field in a dielectric medium. We shall neglect here thermal radiation which is unimportant for the problems of interest to us. If there are no interactions with charged particles the trace in (5.29) reduces then to an average over the ground state (the vacuum of free photons); the form of the function $D^{(o)}_c(\vec{k},\omega)$ is well known from quantum electrodynamics (see Bogolyubov and Shirkov, 1957, and also appendix III):

$$D_c^{(o)}(\vec{k}, \omega) = \frac{1}{(2\pi)^4 (\vec{k}^2 - k_o^2 - i\varepsilon)} . \tag{5.38}$$

In particular, in the non-relativistic approximation (that is, when we neglect the effects of the retardation of the electromagnetic field) we get

$$D_c^{(o)}(\vec{k}, \omega) = \frac{1}{(2\pi)^4 \vec{k}^2} . \tag{5.39}$$

As should be the case, the poles of (5.38) lie at the points $\omega = c|\vec{k}|$. On the other hand, the function (5.39) has no poles in the ω-plane, and is, in general, independent of ω. This is obvious: (5.39) corresponds to the electrostatic approximation, which as a matter of principle excludes the possibility of electromagnetic waves in the dielectric. We note that in that approximation we can for $\alpha = \beta = 0$ neglect the second term on the right-hand side of (5.35) and get thus

$$D_{c,oo}^{(o)}(\vec{k}, \omega) = D_c^{(o)}(\vec{k}, \omega) . \tag{5.40}$$

We draw attention to the fact that, apart from a constant factor, the right-hand side of (5.39) is the three-dimensional Fourier transform of the Coulomb potential $|\vec{x} - \vec{x}'|^{-1}$. This fact is not accidental, as we shall see in section 8.

Chapter II

THE GREEN FUNCTION EQUATIONS OF MOTION

6. EQUATIONS OF MOTION AND HAMILTONIANS

We get the equations for the Green functions by differentiating K_r, K_a, and K_c with respect to x_0 and then using the equations of motion for the operators C_1 and C_2:

$$\frac{\partial C_l}{\partial x_0} = i\,(H'\,C_l - C_l\,H')\,, \qquad l = 1,\ 2\,. \tag{6.1}$$

From (6.1) and the definitions (3.1) to (3.4) and (3.17) we get

$$i\frac{\partial}{\partial x_0}\ll C_1(x)\,|\,C_2(x')\gg_j = -\,\delta(x_0-x_0')\,\langle C_1(x)C_2(x')\rangle - \ll H'C_1(x) - C_1(x)H'\,|\,C_2(x')\gg_j\,, \tag{6.2}$$

$$i\frac{\partial}{\partial x_0}\ll C_1(x)\,|\,C_2(x')\gg_j^{(\pm)} = -\,\delta(x_0-x')\,\langle [C_1(x), C_2(x')]_\pm\rangle - \ll H'C_1(x) - C_1(x)H'\,|\,C_2(x')\gg_j^{(\pm)}\,, \tag{6.3}$$

$$i\frac{\partial K_c(x,x')}{\partial x_0} = -\,\delta(x_0-x_0')\,\langle C_1(x)C_2(x') - \eta C_2(x')C_1(x)\rangle - i\,\langle T\,\{H'C_1(x) - C_1(x)H', C_2(x')\}\rangle\,, \tag{6.4}$$

where j and η are the same as in section 3. One sees from (6.2) to (6.4) the well-known practical advantage of the $K_j^{(\pm)}$ over the K_j: in the first case the delta-function $\delta(x_0-x_0')$ is multiplied into the commutator or the anticommutator of C_1 and C_2. When the time-arguments are the same, these may turn out to be delta-functions in the other variables, and this simplifies the structure of the equations considerably.

Equations (6.2) to (6.4) are convenient for a study of Green functions whenever the wave functions of the corresponding particles satisfy differential equations of the first order in time. This is the case (in the non-relativistic limit) for any particle with a non-vanishing restmass. The electromagnetic and phonon fields are, on the other hand, described by differential equations of the second order in time. It is accordingly convenient to introduce into the Green function equations also second derivatives with respect to the time (see section 7).

If we want to write down (6.2) to (6.4) in all detail, we need to know not only the actual form of C_1 and C_2, but also the Hamiltonian H' of the system. The latter is in the general case of the form

$$H' = H'_{\mathrm{p}} + H_{\mathrm{int}} + H_{\mathrm{f}} + H_{\mathrm{pf}} \,. \tag{6.5}$$

Here H'_{p} is a Hamiltonian which is a sum of terms referring to the individual non-interacting particles which move in some classical, external field and which includes the term $-\mu N$; H_{int} is the Hamiltonian of the direct (usually pairwise) interaction between the particles; H_{f} is the Hamiltonian of the free quantum field (or fields); and H_{pf} is the Hamiltonian of the interaction betwenn the particles and the quantum field (or fields).

We note that, strictly speaking, it should be sufficient to take only the interaction with the quantum fields into account; the direct interaction between the particles could then be obtained as a consequence from the former (in the same way as one can, for instance, obtain the Coulomb interaction in quantum electrodynamics). It is, however, practically more convenient in a number of problems to consider straightaway the direct interaction. This is the case whenever one can neglect the retardation effects of the interactions through the field and when the quantum fields only act through virtual processes while real absorption or emission processes are unimportant.

If we denote by T and V the kinetic and potential energy operators of a particle in a classical external field, we have

$$H'_{\mathrm{p}}(x_0) = \int \mathrm{d}\lambda \, \mathrm{d}\lambda' \, (\lambda \,|\, T+V-\mu \,|\, \lambda') \, a^+(\lambda, x_0) a(\lambda', x_0) \,. \tag{6.6}$$

It may turn out, in particular cases, to be convenient to work in a representation in which the operator $T+V-\mu$ is diagonal. If we denote its eigenvalues by $E(\lambda)$, we have

$$H'_{\mathrm{p}}(x_0) = \int \mathrm{d}\lambda \, E(\lambda) \, a^+(\lambda, x_0) a(\lambda, x_0) \,. \tag{6.7}$$

Let, moreover, the operator of the pairwise direct particle-particle interaction be U. We then have

$$\begin{aligned} H_{\mathrm{int}}(x_0) = {} & \tfrac{1}{2} \int \mathrm{d}\lambda_1 \, \mathrm{d}\lambda_2 \, \mathrm{d}\lambda'_1 \, \mathrm{d}\lambda'_2 \, (\lambda_1, \lambda_2 \,|\, U \,|\, \lambda'_2, \lambda'_1) \\ & \times a^+(\lambda_1, x_0) a^+(\lambda_2, x_0) a(\lambda'_2, x_0) a(\lambda'_1, x_0) \,. \end{aligned} \tag{6.8}$$

In the fermion case when the operators $a(\lambda, x_0)$ and $a(\lambda', x_0)$ anticommute, we must take the form of $(\lambda_1, \lambda_2 \,|\, U \,|\, \lambda'_2, \lambda'_1)$ which is antisymmetrised with respect to the permutation $\lambda_1 \rightleftarrows \lambda_2$ and $\lambda'_1 \rightleftarrows \lambda'_2$ (in the boson case we must take the symmetrised form).

In the coordinate representation most of the off-diagonal elements of U vanish usually, and we have

$$H_{\text{int}}(x_0) = \tfrac{1}{2} \int \mathrm{d}^3\vec{x}\ \mathrm{d}^3\vec{x}'\ a^+(\vec{x})a^+(\vec{x}')\ U(\vec{x}-\vec{x}')\ a(\vec{x}')a(\vec{x})\ . \qquad (6.8a)$$

We note that as the total Hamiltonian is an integral of motion, it is immaterial what value of x_0 we choose: it is only necessary to choose the same value for all terms of (6.5), as the separate terms are, generally speaking, not integrals of motion. The most convenient choice is the value of x_0 occurring as argument in $C_1(x)$ in (6.2) to (6.4).

It is convenient to write down the operators H_f and H_{pf} first of all for the particular cases which we shall consider in the following.

a. *Charged particles in an electromagnetic field.* It is well known from quantum electrodynamics (Bogolyubov and Shirkov 1957) that one can write the Hamiltonian of the free electromagnetic field in the form *

$$H_f(x_0) = -\tfrac{1}{2} \int \mathrm{d}x \sum_\beta g^{\beta\beta} :\left\{\frac{1}{c^2}\left(\frac{\partial A_\beta(x)}{\partial x_0}\right)^2 + \sum_{i=1,2,3}\left(\frac{\partial A_\beta(x)}{\partial x_i}\right)^2\right\}: . \qquad (6.9)$$

The symbol $:\{\ldots\}:$ indicates here that in the corresponding expression all photon creation operators must stand to the left of the annihilation operators. The product ordered in this way is called the normal product (Bogolyubov and Shirkov 1957; see also appendix I).

The Hamiltonian describing the interaction between the field and charged particles is (in the coordinate representation) of the form (Bogolyubov and Shirkov 1957)

$$H_{pf}(x_0) = -e \int \mathrm{d}^3\vec{x}\ a^+(x)\ \gamma^\beta\ a(x)\ A_\beta(x)\ , \qquad (6.10)$$

where the γ are the Dirac matrices. We have not written down here the normal product symbol, since in the problems considered by us there is no unobservable background. We note that, if we are interested only in processes involving virtual photons (and if we neglect quantities of order $1/c$) we can replace (6.10) by the direct Coulomb interaction between the electrons, that is, by an equation of the form (6.8) with the Coulomb potential for U.

b. *Electrons in a phonon field.* We denote by $\xi^+(\nu)$ and $\xi(\nu)$ the operators creating or annihilating phonons of type ν, and by $\omega(\nu)$ their energy (the symbol ν includes both the three components of the quasi-wave vector $\vec{k}$ and the index indicating the branch of the phonon spectrum). The Hamiltonian of the free phonon field will then be

$$H_f(x_0) = \sum\nolimits_\nu \omega(\nu)\ \xi^+(\nu,x_0)\ \xi(\nu,x_0)\ . \qquad (6.11)$$

* When integrated this formula is equivalent to the usual expression $H_f = \tfrac{1}{2}\int (\vec{E}^2 + \vec{H}^2)\ \mathrm{d}^3\vec{x}$.

As always in similar cases, the sum Σ_ν may include an integral over continuous variables which are involved in ν; it is, however, convenient to make the components of $\vec{k}$ discrete by considering the phonon system in a large cube of volume V and imposing the periodicity conditions at the boundaries of the cube.

The Hamiltonian describing the interaction between the phonons and the electrons can be written in the form

$$H_{\mathrm{pf}}(x_0) = -g \sum_{\vec{k},\vec{p},\vec{p}',s} V^{-\frac{1}{2}} \{f(\vec{k})\delta(\vec{p}-\vec{p}'-\vec{k})\xi(\vec{k},x_0)a^+(\vec{p},s,x_0)a(\vec{p}',s,x_0)$$

$$+ f^+(\vec{k})\delta(\vec{p}-\vec{p}'-\vec{k})\xi^+(\vec{k},x_0)a^+(\vec{p}',s,x_0)a(\vec{p},s,x_0)\} . \qquad (6.12)$$

Here $\vec{p}$ and $\vec{p}'$ are the quasi-momenta of the electron in the crystalline lattice, s the spin-coordinate, and the operators ξ and ξ^+ refer to longitudinal (acoustic or optical) phonons. The quantity g is a coupling constant. It has a different form for semi-conductors and for metals (for details see sections 26 and 27). The function $f(\vec{k})$ is different for acoustic and optical phonons; for long-wavelength phonons ($k \to 0$) we have

$$f_{\mathrm{acoust}} = i|\vec{k}| \,/\, [\omega(\vec{k})]^{\frac{1}{2}} , \qquad (6.13)$$

$$f_{\mathrm{opt}} = [\omega(\vec{k})]^{\frac{1}{2}} \,/\, |\vec{k}| . \qquad (6.14)$$

Expression (6.12) corresponds to the simplest approximation where one assumes the electron-phonon interaction to be isotropic, and where one, moreover, does not take Umklapp-processes into account. The generalisation to a more complicated case is not difficult, but we do not need it in this book.

Under well-defined assumptions one can replace (6.12) by a Hamiltonian of the form (6.8), that is, eliminate the explicit mentioning of the phonon field by introducing instead a direct electron-electron interaction (Tolmachev and Tyablikov 1958a). The corresponding operator H_{int} is called the Bardeen Hamiltonian and is of the form

$$H_{\mathrm{int}} = \frac{B}{2V} \sum_{\vec{p},\vec{p}'} a^+(\vec{p},s,x_0)a^+(-\vec{p},-s,x_0)a(-\vec{p}',-s,x_0)a(\vec{p}',s,x_0) , \qquad (6.15)$$

where B is a constant.

We note, moreover, that (6.10) and (6.12) can be written in the same form. Indeed, we can introduce a "quantum field potential" $\phi(\vec{x},x_0)$ (which may still depend on some discrete variables, such as a vector index, which we shall not write down explicitly). In the case of the electromagnetic field $\phi(\vec{x},x_0)$ is represented by the four components $A_\beta(x)$. In the case of the phonon field, we can in (6.12) change to the coordinate representation and then find easily

$$\Phi(\vec{x}, x_0) = (2V)^{-\frac{1}{2}} \sum_{\vec{k}} \{f(\vec{k})\, e^{i(\vec{k}\cdot\vec{x})}\, \xi(\vec{k}, x_0) + f^+(\vec{k})\, e^{-i(\vec{k}\cdot\vec{x})}\, \xi^+(\vec{k}, x_0)\} . \tag{6.16}$$

We have thus in both cases (in the electromagnetic case, the coupling constant g is equal to e)

$$H_{pf}(x_0) = -g \int d^3\vec{x}\; a^+(x)\, \Gamma^{(0)}\, a(x)\, \Phi(x) , \tag{6.17}$$

where

$$\Gamma^{(0)} = \begin{cases} \gamma^\beta & \text{in electrodynamics,} \\ 1 & \text{in the phonon-field case.} \end{cases} \tag{6.18}$$

The quantity $\Gamma^{(0)}$ is called the elementary vertex part. This nomenclature is connected with a special method of diagrammatically depicting the Green function equations (see appendix I).

It is not difficult to generalise all further discussions (sections 7 to 9) also to the more general, non-local case when the matrix $\Gamma^{(0)}$ in (6.17) is no longer diagonal, not only with respect to the spin coordinates, but also with respect to the spatial coordinates (all operators are thus taken at different points in space and the number of integrals in (6.17) is trebled).

The "coordinate" form of writing (6.17) turns out to be very convenient (although, of course, not always) for formulating and studying the equations in terms of functional derivatives (see sections 8 to 10). It is equally applicable to any other field; in particular, we have not specified the tensor dimensionality of Φ and $\Gamma^{(0)}$ (except that the product $\Gamma^{(0)}\Phi$ must clearly be invariant under any symmetry transformation which is peculiar to the system considered).

c. *A spin system in a ferromagnetic.* For the sake of completeness we give here yet another Hamiltonian, which we shall discuss when we consider ferromagnetic phenomena (the Heisenberg Hamiltonian). Let $b^+(\vec{f})$ and $b(\vec{f})$ be the Pauli operators depending on the coordinates of the lattice site $\vec{f}$. Let, moreover, $A(\vec{f}_1 - \vec{f}_2)$ be the exchange integral for electrons on the lattice sites $\vec{f}_1$ and $\vec{f}_2$, and

$$A'(\vec{k}) = \sum_{\vec{f}} A(\vec{f})\, e^{i(\vec{k}\cdot\vec{f})}$$

be its Fourier transform, where $\vec{k}$ is the wave vector.

Let, finally, $\mathcal{H}$ be the magnitude of the external magnetic field and μ_B the Bohr magneton. The Heisenberg Hamiltonian is then of the form

$$H = C + [2\mu_B \mathcal{H} + 2A'(0)] \sum_{\vec{f}} n(\vec{f}) - 2 \sum_{\vec{f}_1,\vec{f}_2} A(\vec{f}_1 - \vec{f}_2) b^+(\vec{f}_1) b(f_2)$$
$$- 2 \sum_{\vec{f}_1,\vec{f}_2} A(\vec{f}_1 - f_2) n(f_1) n(f_2) \ . \qquad (6.19)$$

Here

$$n(\vec{f}) = b^+(\vec{f}) b(\vec{f}) \ , \qquad C = -\tfrac{1}{2} N A'(0) - N \mu_B \mathcal{H} \ ,$$

and N the total number of lattice sites. For a derivation of the Hamiltonian (6.19) we refer to the literature (for instance, Bogolyubov 1949, Bogolyubov and Tyablikov 1949a, b).

7. THE CHAIN OF EQUATIONS FOR THE DOUBLE-TIME GREEN FUNCTIONS *

We shall now write down explicitly (6.2) to (6.4) for some of the simplest Green functions. We shall restrict ourselves here to fermion systems only. The case where a^+ and a are Pauli operators is considered in chapter VII; the change in the results of the present and the subsequent sections for the case of boson systems consists only in a change of signs in some intermediate formulae.

Let us, to begin with, consider a fermion system with direct interactions only. We shall consider the equation for the single-fermion Green function, putting $C_1(x) = a(\lambda, x_0)$ and $C_2(x') = a^+(\lambda', x_0')$. The usual commutation relations are valid for the operators a and a^+ at the same time **

$$[a(\lambda, x_0), a^+(\lambda', x_0)]_+ = \delta(\lambda - \lambda') \ , \qquad [a(\lambda, x_0), a(\lambda', x_0)]_+ = 0 \ . \qquad (7.1)$$

Using (7.1), (6.6), and (6.8) and taking into account the antisymmetry properties of the matrix elements of the operator U (see the discussion of (6.8)) we find easily

$$[H_p'(x_0), a(\lambda, x_0)]_- = \mu\, a(\lambda, x_0) - \int d\lambda' \, (\lambda | T + V | \lambda') \, a(\lambda') \ , \qquad (7.2)$$

$$[H_{int}(x_0), a(\lambda, x_0)]_- = - \int d\lambda' \, d\lambda'' \, d\lambda''' (\lambda, \lambda' | U | \lambda''', \lambda'') a^+(\lambda') a(\lambda'') a(\lambda''') \ . \qquad (7.3)$$

It is clear from (7.1) that in this case it is advantageous to consider together with G_c the functions $G_r^{(+)}$ and $G_a^{(+)}$ (see the discussion of (6.2) to (6.4)). Indeed, the first terms on the right-hand sides of (6.3) and (6.4) become then delta-functions both in $x_0 - x_0'$ and in $\lambda - \lambda'$.

* See Bogolyubov and Tyablikov 1959.

** As always in such cases the symbol $\delta(\lambda - \lambda')$ denotes a product of Dirac delta-functions for the continuous variables and Kronecker deltas for the discrete variablss involved in λ.

The equations for $G^{(-)}_{r,a}$ and $G_{r,a}$ are now somewhat more complicated. The final result, for instance, for the energy spectrum of the system is, of course, the same, whichever of the equations (6.2) to (6.4) is used. We are here considering only a formal simplification for the calculations. We introduce "two-particle" Green functions, putting

$$G^{(+)}_{2,r}(\lambda', \lambda'', \lambda''', x_0; \lambda_1, x_0') = i\,\theta(x_0 - x_0') \langle [a^+(\lambda', x_0) a(\lambda'', x_0) a(\lambda''', x_0), a^+(\lambda_1, x_0')]_+ \rangle , \quad (7.4)$$

$$G^{(+)}_{2,a}(\lambda', \lambda'', \lambda''', x_0; \lambda_1, x_0') = -i\,\theta(x_0' - x_0) \langle [a^+(\lambda', x_0) a(\lambda'', x_0) a(\lambda''', x_0), a^+(\lambda_1, x_0')]_+ \rangle , \quad (7.5)$$

$$G_{2,c}(\lambda', \lambda'', \lambda''', x_0; \lambda_1, x_0') = i \langle T\,\{a^+(\lambda', x_0) a(\lambda'', x_0) a(\lambda''', x_0) a^+(\lambda_1, x_0')\} \rangle . \quad (7.6)$$

These functions are special cases of the general two-particle Green functions which depend on four time-coordinates. Another special case was given by (5.24). Equations (6.3) and (6.4) for the functions $G^{(+)}_r$, $G^{(+)}_a$, and G_c are now of the form

$$i\frac{\partial}{\partial x_0} G(\lambda, x_0; \lambda', x_0') + \mu\, G(\lambda, x_0; \lambda', x_0') - \int d\lambda_1 (\lambda | T+V | \lambda_1) G(\lambda_1, x_0; \lambda', x_0') - \int d\lambda_1\, d\lambda_2\, d\lambda_3 (\lambda, \lambda_1 | U | \lambda_2, \lambda_3) G_2(\lambda_1, \lambda_2, \lambda_3, x_0; \lambda', x_0') = -\delta(x_0 - x_0')\,\delta(\lambda - \lambda') . \quad (7.7)$$

In particular, we get for a system with spin-independent forces in the coordinate representation

$$\left\{ i\frac{\partial}{\partial x_0} + \mu - T_{\vec{x}} - V(\vec{x}) \right\} G(x, x') - \int d^3\vec{x}''\, U(\vec{x} - \vec{x}'')\, G_2(\vec{x}'', \vec{x}'', \vec{x}, x_0; \vec{x}', x_0') = -\delta(x - x') , \quad (7.7a)$$

where $U(\vec{x})$ is the usual interaction potential energy with $U(\vec{x}) = U(-\vec{x})$. We have deliberately dropped all indices of the functions G and G_2, as the equations connecting $G^{(+)}_r$ with $G^{(+)}_{2,r}$, $G^{(+)}_a$ with $G^{(+)}_{2,a}$, or G_c with $G_{2,c}$ are all completely identical.

For a boson system we get exactly the same equations, but instead of the functions $G^{(+)}_{r,a}$ and $G^{(+)}_{2,r,a}$ we must take $G^{(-)}_{r,a}$ and $G^{(-)}_{2,r,a}$. The same applies also to the equations given in the following, such as (7.10).

On the left-hand side of (7.7) there occurs apart from the required Green function G also the "two-particle" function G_2. One ob-

tains an equation for this function by a completely analogous method, and one sees easily that in that equation there occurs apart from G_2 also a "three-particle" Green function G_3 which contains six operators a^+ and a under the averaging sign. Continuing this process we get an infinite chain of coupled equations. We must, of course, consider apart from (7.7) and so on also the chain of the conjugate equations which are obtained by differentiating G, G_2, ... with respect to x_0' (and not with respect to x_0). As a rule, we shall in the following not mention this fact explicitly, but only imply it. In the literature (Bogolyubov 1947, 1949) one finds a chain of equations for particular distribution functions which is completely similar to the left-hand sides of the chain of equations for the Green functions, as far as their structure is concerned. The difference between the two cases consists in the fact that now the functions we are trying to find depend on two time coordinates and that now the system is not homogeneous. This last fact is connected with the circumstance that the functions considered here have singularities when the two time coordinates are the same, which is just the circumstance which enabled us in sections 4 and 5 to extend the definition of the spectral functions to the whole of the complex plane. We shall see that this, indeed, makes the solution for actual problems considerably easier. The occurrence of such chains of equations is typical for any method of solving the many-body problem and is, apparently, inevitable in one form or another. Indeed, it reflects only the impossibility to isolate exactly any group of particles from the remainder of the system when there are interactions present. An exact solution of such infinite systems of equations is, as a rule, impossible, and one must have recourse to some approximation method to "decouple" the chain (for instance, by assuming that one may express the n-th Green function in a well-defined way in terms of the lower order Green functions). It is at this juncture that various approximations come into force; there is no sense in considering these in the general form, but only when applied to different specific problems (see chapters IV to VII).

We see from (7.7) that $G_r^{(+)}$, $G_a^{(+)}$, and G_c are solutions of the same set of equations, but with different boundary conditions, as far as the time coordinate is concerned. The form of these boundary conditions can formally be obtained from the definitions (3.1) to (3.4) and (3.17); it is, however, not always convenient to formulate these directly as conditions imposed upon the required functions as $x_0 - x_0' \to \pm\infty$ or as $x_0 - x_0' \to 0$. In practice, however, such a direct formulation is not necessary, as it is equivalent to a particular choice of the spectral representations of the dispersion relations obtained in sections 3 to 5. We saw, indeed, for instance from the derivation of (3.7) and (3.8) that a particular combination of θ-functions depending on $x_0 - x_0'$ predetermines a particular rule for going round the poles in integrands (for details see section 10). It is thus suffi-

cient, if one wishes to satisfy the boundary conditions, to require that the required function admits a spectral representation of the appropriate form. In practice it will be most convenient to use the dispersion relations (4.7), (4.8), or (4.10).

We note, finally, that (7.7) differs from the equation of motion for the matrix elements of the operator $a(\lambda, x_0)$ in the Heisenberg representation only through the occurrence of an inhomogeneous term on the right-hand side. This is not accidental. It follows from the structure of the expressions (3.1) to (3.4) and (3.17) which differ from the average $<C_1(x)\,C_2(x')>$ only by the occurrence of discontinuous factors, and differentiating them leads to the delta-function inhomogeneity. This fact is also the one which allows us to call (3.1) to (3.4) and (3.17) Green functions. We are, indeed, dealing here with Green functions (for the Schrödinger equation, the Maxwell equations, and so on) in the usual mathematical sense of this term.

The situation is completely analogous when there are interactions between the particles and quantum fields. (We shall use here the coordinate representation.) From (7.1) and (6.17) we have

$$[H_{\mathrm{pf}}(x_0), a(\vec{x}, x_0)]_- = g\,\Gamma^{(0)}\,a(x)\,\Phi(x)\,. \tag{7.8}$$

We now introduce a "mixed" fermion-boson Green function of the form

$$R_{\mathrm{c}}(s, \vec{x}, x_0; s', \vec{x}', x_0') = \mathrm{i}\,<T\,\{a(s,x)a^{+}(s',x')\Phi(x)\}>\,; \tag{7.9}$$

one can introduce functions $R^{(+)}_{\mathrm{r,a}}$ by analogy with (3.1) to (3.4).

We get then for the functions $G^{(+)}_{\mathrm{r}}$, $G^{(+)}_{\mathrm{a}}$, and G_{c} the equation

$$\left(\mathrm{i}\,\frac{\partial}{\partial x_0} + \mu\right) G(s,x;s',x') - (s\,|\,T_{\vec{x}} + V(\vec{x})\,|\,s'')\,G(s'',x;s',x') + g\,\Gamma^{(0)}(s,s'')\,R(s'',x;s',x') = -\,\delta(x_0 - x_0')\,\delta(\vec{x}-\vec{x}')\,\delta_{ss'}\,. \tag{7.10}$$

We have here taken into account that $T_{\vec{x}}$ is in the coordinate representation a differential operator (the Dirac or the Schrödinger operator, depending on the character of the problem considered), while the matrix $(\vec{x}\,|\,V\,|\,\vec{x}')$ is diagonal. We have, however, not assumed that V is diagonal in the spin variables, retaining thus the possibility of spin-interactions. We shall, as a rule, not explicitly mention the spin indices, but bear in mind the appropriate matrix multiplication.

We must in the present case introduce apart from the single-fermion Green function also a single-boson Green function, defining it by a relation similar to (5.29):

$$D_{\mathrm{c}}(x,x') = -\,\mathrm{i}\,<T\,\{\Phi(x)\Phi(x')\}>\,, \tag{7.11}$$

and similar equations for $D^{(-)}_{\mathrm{r}}$, $D^{(-)}_{\mathrm{a}}$, ...

Using (6.1) and the commutation relations for the $\Phi(x)$ we find easily the equation of motion for D_{c}. We consider first of all the

specific examples of the interaction of fermions with the electromagnetic field and with the field of acoustic phonons.

In the first case we have for the commutation relations for the operators $A_\alpha(x)$, $A_\beta(x')$ at the same time the relation (see appendix I)

$$\begin{aligned} &[A_\alpha(\vec{x},x_0),\ A_\beta(\vec{x}',x_0)]_- = 0\ , \\ &[\frac{\partial A_\alpha(\vec{x},x_0)}{\partial x_0}\ ,\ A_\beta(\vec{x}',x_0)]_- = i\ c^2\ g_{\alpha\beta}\ \delta(\vec{x}-\vec{x}')\ , \\ &[\frac{\partial A_\alpha(\vec{x},x_0)}{\partial x_i}\ ,\ A_\beta(\vec{x}',x_0)]_- = 0\ . \end{aligned} \tag{7.12}$$

One verifies easily, by using (6.9), (6.10), and (7.12), that (6.1) applied to the operator $A_\beta(x)$ gives an identity $\partial A_\beta/\partial x_0 = \partial A_\beta/\partial x_0$ (which also indicates that in this case the equation of motion for A_β and hence for D_c is not first order, but higher order, in the time). Applying then (6.1) to the operator $\partial A_\alpha(x)/\partial x_0$ and again using the commutation relations (7.12) and (6.9) and (6.10), we find easily

$$\frac{1}{c^2}\ \frac{\partial^2 A_\alpha(x)}{\partial x_0^2}\ -\ \nabla^2_{\vec{x}}\ A_\alpha(x) = -\ e\ g_{\alpha\beta}\ a^+(x)\ \gamma^\beta\ a(x)\ . \tag{7.13}$$

This is, as one should have expected, the usual d'Alembert equation with the quantum current on the right-hand side. From (7.11) and (7.12) we get for $D_c(x,x')$

$$\frac{\partial D_{c,\alpha\beta}(x,x')}{\partial x_0} = -\ i\ \langle T\ \left\{\frac{\partial A_\alpha(x)}{\partial x_0}\ ,\ A_\beta(x')\right\}\rangle\ ,$$

$$\frac{\partial^2 D_{c,\alpha\beta}(x,x')}{\partial x_0^2} = c^2\ g_{\alpha\beta}\ \delta(x-x')\ -\ i\ \langle T\ \left\{\frac{\partial^2 A_\alpha(x)}{\partial x_0^2}\ ,\ A_\beta(x')\right\}\rangle\ .$$

Using (7.13), we get, finally:

$$\left(\frac{1}{c^2}\ \frac{\partial^2}{\partial x_0^2}\ -\ \nabla^2_{\vec{x}}\right) D_{c,\alpha\beta}(x,x')\ -\ i\ e\ g_{\alpha\lambda}\ \langle T\ \{a^+(x)\ \gamma^\lambda\ a(x)\ A_\beta(x')\}\rangle$$

$$= g_{\alpha\beta}\ \delta(x-x')\ . \tag{7.14}$$

We note that if we wish to verify (7.14) for a particular form of $D_c(x,x')$ we must tread warily. For instance, if we substitute for the free field here (5.30) and (5.35) and perform the differentiation under the integral sign we may get on the right-hand side additional terms of the kind $\delta''(\vec{x}-\vec{x}')$. This is connected with the singularity of the T-product when the time arguments are the same (or, which comes to the same, with a divergence of the integral we obtain) and indicates merely the inadmissability of the procedure.

Let us now turn to the second case: the interaction of electrons with acoustic phonons. The commutation relations for the operators

$\Phi(x)$ are easily found by using (6.16) and the commutation relations for the ξ and ξ^+:

$$[\xi(\vec{k}),\ \xi^+(\vec{k}')]_- = \delta(\vec{k}-\vec{k}')\ ,\qquad [\xi(\vec{k}),\ \xi(\vec{k}')]_- = 0\ . \tag{7.15}$$

We get in this way

$$\begin{aligned} &[\Phi(\vec{x},x_0),\ \Phi(\vec{x}',x_0)]_- = 0\ ,\\ &[\Phi(\vec{x}',x_0),\ \frac{\partial\Phi(x,x_0)}{\partial x_0}]_- = -\,i\,\nabla^2_{\vec{x}}\,\delta(\vec{x}-\vec{x}')\ . \end{aligned} \tag{7.16}$$

Using (6.1), (6.17), (6.11), and (7.16) to evaluate the derivative $\partial\Phi(x)/\partial x_0$ we can again check that (6.1) when applied to $\Phi(x)$ in this case leads to the identity $\partial\Phi/\partial x_0 = \partial\Phi/\partial x_0$. If we then apply (6.1) to the operator $\partial\Phi(x)/\partial x_0$, we get

$$\begin{aligned} \frac{\partial^2\Phi(x)}{\partial x_0^2} = &-V^{-\frac{1}{2}}\sum_{\vec{k}}\omega^2(\vec{k})\,\{f(\vec{k})\,e^{i(\vec{k}.\vec{x})}\,\xi(\vec{k},x_0) + f^+(\vec{k})\,e^{-i(\vec{k}.\vec{x})}\,\xi(\vec{k},x_0)\}\\ &- g\,\nabla^2_{\vec{x}}\,a^+(x)\,\Gamma^{(0)}\,a(x)\ . \end{aligned} \tag{7.17}$$

The first term on the right-hand side of (7.17) can be transformed by introducing the operator $\omega^2(-i\nabla_{\vec{x}})$, defined by

$$\omega^2(-i\nabla_{\vec{x}})\,e^{i(\vec{k}.\vec{x})} = \omega^2(\vec{k})\,e^{i(\vec{k}.\vec{x})}\ . \tag{7.18}$$

Since $\omega(\vec{k})$ is an even function, the term considered can be written as

$$-\,\omega^2(-i\nabla_{\vec{x}})\,\Phi(x)\ . \tag{7.19}$$

Using (7.16), (7.17), and (7.19), we find immediately an equation for $D_c(x,x')$:

$$\begin{aligned} &\frac{\partial^2 D_c(x,x')}{\partial x_0^2} + \omega^2(-i\nabla_{\vec{x}})D_c(x,x') - ig\nabla^2_{\vec{x}}\,\langle T\,\{a^+(x)\,\Gamma^{(0)}\,a(x)\,\Phi(x')\}\rangle\\ &\qquad = \nabla^2_{\vec{x}}\,\delta(x-x')\ . \end{aligned} \tag{7.20}$$

One can now easily write down the equation of motion for $D_c(x,x')$ in the general form which is valid for any boson field * interacting with fermions according to the law (6.17). To do this we note that the differential operators acting upon $D_c(x,x')$ on the left-hand sides of (7.14) and (7.20) define the equations of motion of the corresponding free fields; on the other hand, the factors (generally speaking operators) in front of the δ-function and in front of the averages of the triple products are determined both by the commutation relations for the field operators $\Phi(x)$ and by the form of the interaction Hamiltonian. From the structure of the equations it is clear that the same will also

* We have in mind fields, the number of quanta of which are not conserved (this is clearly evident from (6.17)).

be true in the general case (only the explicit form of the above-mentioned operators depends on the specific nature of the field). We shall denote the differential operator occurring in the equations of motion for the free boson field by $L(x) = (\partial^2/\partial x_0^2) - L(\vec{x})$ and the factor of the δ-functions and the triple products by $f(\vec{x})$. We introduce, furthermore, one more "mixed" Green function

$$Q_c(s, s', x, x') = i \langle T \{ a(s, x) a^+(s', x), \Phi(x') \} \rangle . \qquad (7.21)$$

(It differs from R_c by a different distribution of the time arguments over Φ and a^+; similarly we can introduce $Q_r^{(-)}$, $Q_a^{(-)}$, and so on.)

We can then write the general equation for $D_c(x,x')$ in the form

$$L(x)\, D_c(x,x') + g f \mathrm{Tr}\, \Gamma^{(0)}\, Q_c(x,x') = f\, \delta(x-x') . \qquad (7.22)$$

The trace is taken here over the spin variables; the quantities f, $\Gamma^{(0)}$, and Q_c may be tensor quantities. In accordance with (7.14) and (7.20), the operator f has in the electromagnetic and the phonon case the form c^2 and $\nabla_{\vec{x}}^2$, respectively (in electrodynamics the "unit" matrix is $g_{\alpha\beta}$).

One gets similar equations for the functions $D_{r,a}^{(-)}$ and $D_{r,a}^{(-)}$.

In those cases where f is a differential operator, (7.22) differs formally from the usual equation for the Green function, as it contains on the right-hand side not simply a δ-function, but its derivatives. One can, however, easily obtain also an equation of the usual kind, by putting

$$D_c(x,x') = f\, \Delta_c(x,x') , \qquad (7.23)$$

where $\Delta_c(x,x')$ is a new function. Using (7.22) and (7.23) we get for it

$$L(x)\, \Delta_c(x,x') + g\, \mathrm{Tr}\, \Gamma^{(0)}\, Q_c(x,x') = \delta(x-x') . \qquad (7.24)$$

It would in this case thus be more correct to call not D_c but the auxiliary quantity Δ_c the Green function; the function D_c is obtained from Δ_c by the action of the differential operator f. It is clear that the spectral representations and dispersion relations established earlier for D_c are valid also for Δ_c. We shall, however, continue to call D_c a "Green function" bearing in mind that this can not lead to any essential misunderstanding.

One can easily connect the function Δ_c for the phonon field with the averages of the operators ξ and ξ^+. Using (6.13), (6.16), and (7.23) we get, for example, for acoustic phonons

$$\Delta_c(x,x') = \frac{i}{2V} \sum_{\vec{k}} \omega^{-1}(\vec{k})\, e^{i(\vec{k}\cdot\vec{x}-\vec{x}')} \langle T \{ \xi(\vec{k}, x_0)\, \xi^+(\vec{k}, x_0')$$

$$+ \xi^+(-\vec{k}, x_0) \xi(-\vec{k}, x_0') - \xi(\vec{k}, x_0) \xi(-\vec{k}, x_0') - \xi^+(-\vec{k}, x_0) \xi^+(\vec{k}, x_0') \} \rangle . \qquad (7.25)$$

One sees easily that this quantity has not merely an auxiliary value, but has also an independent use: in this case the right-hand side of

(6.12) is, apart from a factor $g\rho^{\frac{1}{2}}$ (ρ: crystal density), the divergence of $\vec{u}$, the displacement vector of the lattice atoms from their equilibrium position. Expression (7.25) determines accordingly the time-correlation function and (when $x_0' = x_0$) the average of the product of the longitudinal components of $\vec{u}$.

Sometimes, for instance, when we evaluate the thermodynamic potential of the phonons, it turns out to be convenient to introduce instead of (7.11) directly the Green function involving the operators ξ and ξ^+ themselves, by putting

$$F_c(\vec{k},t) = -i\langle T\{\xi(\vec{k},x_0)\,\xi^+(\vec{k},x_0')\}\rangle , \qquad (7.26)$$

and similarly for $F_{r,a}^{(-)}$.

For a determination of the energy spectrum of the system, the function F_c gives the same result as D_c and similar spectral representations are valid for it. The equations for the functions F_c, $F_r^{(-)}$, and $F_a^{(-)}$ are obtained in the same way as the earlier equations.

One can also obtain by a similar method equations for the "mixed" Green functions R and Q. In these equations enter Green functions of even higher order, that is, as in the case of direct interactions we obtain here, generally speaking, an infinite set of coupled equations. The most convenient way to formulate boundary conditions for these equations is by using dispersion relations such as (4.7), (4.8), and (4.10).

8. EQUATIONS IN TERMS OF FUNCTIONAL DERIVATIVES *

When one solves in actual cases sets of equations such as (7.7), (7.10), or (7.22) one is always led to some "decoupling" of the chain by using some kind of approximation. This is a reason why it is useful to have different representations of the equations to be studied. In the present section it will be shewn for the causal Green functions that equations such as (7.10) and (7.22) can be written in a very simple form, if we introduce functional derivatives of the required functions with respect to some auxiliary arguments. We give the calculations explicitly for fermion systems; we shall indicate later (in section 9) what changes have to be made when we change to a boson system. Without going beyond a "double-time" frame-work, one can also write the equations for the retarded and advanced Green functions in terms of functional derivatives.

Let us first of all turn to (7.10) and consider rather carefully the function $R_c(x,x')$ of (7.9) occurring there (we shall not write down explicitly spin and other discrete variables, assuming all quantities to be appropriate matrices):

* See Kogan (1960), Klein and Prange (1958a), and Bonch-Bruevich and Kogan (1960).

$$R_c(x,x') = i\,\langle T\,\{a(x)a^+(x')\Phi(x)\}\rangle .$$

The problem consists in writing this quantity as some operation acting upon G_c (or upon functions connected with it). To do this we introduce (purely formally)

$$G_c(x,x';J) = \frac{i}{\langle S\rangle}\langle T\,\{a(x)a^+(x')S\}\rangle , \tag{8.1}$$

$$R_c(x,x';J) = \frac{i}{\langle S\rangle}\langle T\,\{a(x)a^+(x')\Phi(x)S\}\rangle , \tag{8.2}$$

$$S = T\,\{\exp i\int d^3\vec{z}\int_{-\infty}^{+\infty} dz_0\, J(z)\,\Phi(z)\} . \tag{8.3}$$

Here, J is some classical function which possesses such transformation properties that the invariance of the product $J\Phi$ under those symmetry transformations, which are allowed in the given system, is guaranteed (for instance, in electrodynamics J is a four-vector with components J^0, J^i, where $J_0 = \rho$ is the "classical external charge density", and $\vec{J}$ the "classical external current density" vector, divided by c).

Clearly we have

$$G_c(x,x') = \lim_{J\to 0} G_c(x,x';J) , \qquad R_c(x,x') = \lim_{J\to 0} R_c(x,x';J) ,$$

and

$$R_c(x,x';J) = -\frac{i}{\langle S\rangle}\frac{\delta\{\langle S\rangle G_c(x,x';J)\}}{\delta J(x)}$$

$$= -i\frac{\delta G_c(x,x';J)}{\delta J(x)} - i\,G_c(x,x';J)\frac{\delta \ln\langle S\rangle}{\delta J(x)} . \tag{8.4}$$

One obtains easily the equation for the function $G_c(x,x';J)$ taking into account that the operators Φ and a taken at the same time commute with one another by definition. Substituting (8.4) into (7.10) we get

$$\left(i\frac{\partial}{\partial x_0} + \mu\right) G_c(x,x';J) - [T_{\vec{x}} + V(\vec{x})]\,G_c(x,x';J)$$

$$- i g\,\Gamma^{(0)}\frac{\delta \ln\langle S\rangle}{\delta J(x)} G_c(x,x';J) - i g\,\Gamma^{(0)}\frac{\delta G_c(x,x';J)}{\delta J(x)} = -\delta(x-x') . \tag{8.5}$$

The functional derivative $-i\,\delta \ln\langle S\rangle/\delta J(x)$ which occurs here has a very clear physical meaning: it determines (as $J \to 0$) the average (both in the quantum-mechanical, and in the thermodynamic case) potential of the quantum field $\Phi(x)$.

Indeed,

$$-i\frac{\delta \ln\langle S\rangle}{\delta J(x)} = \frac{1}{\langle S\rangle}\langle T\,\{\Phi(x)\,S\}\rangle \xrightarrow[J\to 0]{} \langle\Phi(x)\rangle \equiv \tilde{\Phi}(x) . \tag{8.6}$$

Accordingly we put formally

$$\tilde{\Phi}(x;J) = -\,\mathrm{i}\,\frac{\delta \ln \langle S\rangle}{\delta J(x)}\,. \tag{8.7}$$

Equation (8.5) then becomes (the arguments $y,z,\ldots$ are used equivalently with x and x')

$$\{\mathrm{i}\,\frac{\partial}{\partial x_0} + \mu - T_{\vec{x}} - V(x) + g\,\Gamma^{(0)}\,\tilde{\Phi}(x;J)\}\,G_c(x,x';J) - \mathrm{i}\,g\,\Gamma^{(0)}\,\frac{\delta G_c(x,x';J)}{\delta J(x)} = -\,\delta(x-x')\,. \tag{8.8}$$

One can transform (7.22) in exactly the same way. If we consider D_c and Q_c as functionals of J (constructed in the same way as (8.1) and (8.2)) we get

$$Q_c(x,x';J) = -\,\frac{\mathrm{i}}{\langle S\rangle}\,\frac{\delta\langle S\rangle G_c(x,x;J)}{\delta J(x')} = -\,\mathrm{i}\,\frac{\delta G_c(x,x;J)}{\delta J(x')} + G_c(x,x;J)\,\tilde{\Phi}(x';J)\,. \tag{8.9}$$

We thus get for (7.22)

$$L(x)\mathfrak{D}_c(x,x';J) + g\,f\,\mathrm{Tr}\,\Gamma^{(0)}\,G_c(x,x;J)\,\tilde{\Phi}(x';J) + \mathrm{i}\,\tilde{\Phi}(x';J)fJ(x) - \mathrm{i}\,g\,f\,\mathrm{Tr}\,\Gamma^{(0)}\,\frac{\delta G_c(x,x;J)}{\delta J(x')} = f\,\delta(x-x')\,. \tag{8.10}$$

In a similar way we get instead of (7.24), introducing the function $\Delta_c(x,x';J)$ by analogy with (7.23):

$$L(x)\Delta_c(x,x';J) + g\,\mathrm{Tr}\,\Gamma^{(0)}\,G_c(x,x;J)\tilde{\Phi}(x';J) + \mathrm{i}\,\tilde{\Phi}(x';J)J(x) - \mathrm{i}\,g\,\mathrm{Tr}\,\Gamma^{(0)}\,\frac{\delta G\ (x,x;J)}{\delta J(x')} = \delta(x-x')\,. \tag{8.10a}$$

In particular, we get for the single-photon Green function

$$(\frac{1}{c^2}\,\frac{\partial}{\partial x_0^2} - \nabla^2_{\vec{x}})\,D_{c,\alpha\beta}(x,x';J) + e\,g_{\alpha\lambda}\,\mathrm{Tr}\,\gamma^\lambda\,G_c(x,x;J)\,\tilde{A}_\beta(x';J) + \mathrm{i}\,g_{\alpha\lambda}J^\lambda(x)\,\tilde{A}_\beta(x';J) - \mathrm{i}\,e\,g_{\alpha\lambda}\,\mathrm{Tr}\,\gamma^\lambda\,\frac{\delta G_c(x,x;J)}{\delta J^\beta(x')} = g_{\alpha\beta}\,\delta(x-x')\,. \tag{8.11}$$

If the system is spatially uniform and if $J = 0$ we can drop the second and third term on the left-hand side of (8.11) as the potential must be independent of $\vec{x}$ in a uniform system, and a constant potential can, of course, always be assumed to be equal to zero. The same applies also to the general relation (8.10).

We note that the "external current density" J in (8.3) and subsequent equations has a purely formal meaning, and it must be put equal to zero after the functional derivatives have been evaluated. Without mentioning this explicitly we shall in the following always

assume this operation to have been performed. In the case of a system of charged particles, however, J^β enters into the equation for the average potential $\widetilde{A}_\beta(x;J)$ as an actual classical four-current density which produces the given field. Indeed, by using (8.3) and (8.7) we get

$$\frac{1}{c^2}\frac{\partial^2 \widetilde{A}_\beta(x)}{\partial x_0^2} - \nabla_x^2 \widetilde{A}_\beta(x) = - g_{\beta\beta} J_\beta(x) - i e g_{\beta\beta} \operatorname{Tr} \gamma^\beta G_c(x,x) \quad (8.12)$$

(no summation over β). In particular, in the non-relativistic approximation (and neglecting retardation effects) we get for the average scalar potential $\widetilde{\varphi}$ ($= - \widetilde{A}_0$), bearing in mind the connexion (5.4) between $G_c(x,x)$ and the particle concentration $n(x)$:

$$\nabla_x^2 \widetilde{\varphi} = - \rho(x) - e\, n(x) . \quad (8.13)$$

We can thus use (8.12) and (8.13) to evaluate the average potential which is produced by a given classical four-current density. Strictly speaking we should then also evaluate the single-fermion Green function taking the given potential into account. This means that we must assume that in (8.8) $\widetilde{\Phi}(x;J) \neq 0$ when $J = 0$, while the function J in (8.3) must be considered to be the deviation of the classical four-current density from its true value.

In conclusion we draw attention to an important relation between the D_c and the average potential $\widetilde{\Phi}$. We remember the definition (8.7) of the average potential, and take the variation of this quantity with respect to $J(x')$. Using (7.11), we find then easily

$$D_c(x,x') + \widetilde{\Phi}(x)\,\widetilde{\Phi}(x') = - \frac{\delta \widetilde{\Phi}(x)}{\delta J(x')} . \quad (8.14)$$

When applied to the electromagnetic field this equation gives us just the physical meaning of (5.37): only by virtue of (5.37) is (8.14) the same as the usual Lorentz condition imposed upon the components of the four-potential:

$$\frac{1}{c}\frac{\partial \widetilde{A}_0(x)}{\partial x_0} - \frac{\partial \widetilde{A}_i(x)}{\partial x_i} = 0 . \quad (8.15)$$

When, for instance in the case of a spatially uniform system, the second term on the left-hand side of (8.14) is absent, this equation demonstrates explicitly the role of the Green function as a classical "influence function" determining the change of the potential when external sources occur. We have in view, of course, uniformity when there are no external classical sources (or - in electrodynamics - when there are no field sources beyond the compensating charge). Sometimes (8.14) is applied (without the second term) to define the single-boson Green function:

$$D_c'(x,x';J) = - \frac{\delta \Phi(x;J)}{\delta J(x')} . \quad (8.16)$$

This definition is equivalent to (7.11) only, when $\tilde{\Phi} = 0$ (this is the reason why we have put a prime on D_C on the left-hand side of (8.16)); when $\tilde{\Phi} \neq 0$ the functions D_C and D'_C are different (see (8.14)).

In an approximation which is linear in $\tilde{\Phi}(x)$ (sufficiently weak field) (8.16) allows us to express $\tilde{\Phi}$ immediately in terms of J:

$$\tilde{\Phi}(x;J) = -\int dx'\, D'_C(x,x';0)\, J(x') \,. \tag{8.17}$$

It follows, in particular, from this equation that $g \int D'_C(x,x')\, dx'_0$ for $\vec{x}' = 0$ is the potential of a static point "charge" * at the point $\vec{x}' = 0$ (compare the discussion following (5.40)). This fact suggests the possibility to replace any direct (pair-)interaction between particles by an interaction between the particles and a quantised boson field. This problem is discussed in detail in section f of appendix I where we shew under what conditions this substitution is indeed possible.

One can easily check that the equation for D'_C is the same as (8.10), provided we drop there the second and third term on the left-hand side, that is, provided it does not contain the potential $\Phi(x)$ and the current J explicitly. One verifies, for instance, easily that a variation of (8.12) with respect to $J^\beta(x')$ gives (8.11), but without the second and third term on the left-hand side. For this reason it is sometimes more convenient to use D'_C rather than D_C (this is, for instance, the case when we wish to evaluate the average potential in a spatially uniform system of charged particles; see section 21). The dispersion relations of sections 4 and 5 are, on the other hand, derived explicitly for D_C and not for D'_C. Most often, however, we consider uniform systems, and then there is no difference between D_C and D'_C. In the following we shall always write down the equations for D'_C, bearing in mind that they are the same as those for D_C, whenever D_C is of interest.

The chain of equations for the case of a system with direct interactions can also easily be written as a set of equations involving functional derivatives. Indeed, we have by definition

$$G_C(x,x') = \mathrm{i}\ \mathrm{Trace}\ e^{\beta\Omega - \beta H'}\, T\, \{a(x)a^+(x')\} \,. \tag{8.18}$$

We introduce the functional

$$G_C(x,x';F) = \frac{\mathrm{i}}{\langle S\rangle} \langle T\, \{a(x)a^+(x')S\}\rangle \,, \tag{8.19}$$

with $$S = T\, \{\exp \mathrm{i} \int d\lambda\, d\lambda'\, dx_0\, F(\lambda,\lambda';x_0)\, a^+(\lambda,x_0)a(\lambda',x_0)\} \,. \tag{8.20}$$

We also introduce by analogy with (8.7) the quantity

$$\Psi(\lambda,\lambda';x_0) = -\mathrm{i}\, \frac{\delta \ln \langle S\rangle}{\delta F(\lambda,\lambda';x_0)} \,. \tag{8.21}$$

* The word "charge" is put here within quotes as we may be dealing not only with electrodynamic interactions.

We check easily, by performing the variation that

$$G_{2,c}(\lambda_1,\lambda_2,\lambda_3,x_0;\lambda',x_0') = -\,i\,\frac{\delta G_c(\lambda_3,x_0;\lambda',x_0')}{\delta F(\lambda_1,\lambda_2;x_0)} + \Psi(\lambda_1,\lambda_2;x_0)\,G_c(\lambda_3,x_0;\lambda',x_0') \,. \qquad (8.22)$$

We get thus from (7.7)

$$\left(i\frac{\partial}{\partial x_0}+\mu\right) G_c(\lambda,x_0;\lambda',x_0') + \int d\lambda_1\, F(\lambda,\lambda_1;x_0)\, G_c(\lambda_1,x_0;\lambda',x_0') - \int d\lambda_1(\lambda|T+V|\lambda_1)\, G_c(\lambda_1,x_0;\lambda',x_0') - \int d\lambda_1\, d\lambda_2\, d\lambda_3((\lambda,\lambda_1|U|\lambda_3,\lambda_2) \times \left\{-\,i\,\frac{\delta G_c(\lambda_3,x_0;\lambda',x_0')}{\delta F(\lambda_1,\lambda_2;x_0)} + \Psi(\lambda_1,\lambda_2;x_0)\,G_c(\lambda_3,x_0;\lambda',x_0')\right\} = -\,\delta(x-x') \,. \qquad (8.23)$$

The quantity $\Psi(\lambda,\lambda';x_0)$ has a clear physical meaning. Indeed, we get from (8.20) and (8.21)

$$\Psi(\lambda,\lambda';x_0) = \frac{1}{\langle S\rangle}\langle T\,\{a^+(\lambda,x_0)a(\lambda',x_0)\,S\}\rangle \xrightarrow[F\to 0]{} \rho_1(\lambda,\lambda';x_0) \,, \qquad (8.24)$$

where ρ_1 is the first density matrix, defined by (1.9).

We note that through its definition (7.6) the function $G_{2,c}(\lambda_1,\lambda_2,\lambda_3,x_0;\lambda',x_0')$ is antisymmetric (or symmetric, if we are dealing with a boson system) with respect to an interchange of λ_2 and λ_3. This property is not explicitly evident on the right-hand side of (8.22), and this might lead to well-known complications when we evaluate the quantities which occur there by some approximate method. This is not important when we apply it to (8.23) as $G_{2,c}$ occurs there only multiplied by the function $(\lambda,\lambda_1|U|\lambda_3,\lambda_2)$ and this function was shewn to possess the necessary symmetry properties. There may, however, arise complications when we change over to the coordinate representation, as in (7.7a) instead of the complete matrix there occurs the simple potential interaction energy $U(\vec{x}-\vec{x}'')$. It is therefore in this case advisable to symmetrise (or antisymmetrise) the right-hand side of (8.22) explicitly, putting

$$G_{2,c}(\vec{x}'',\vec{x}'',\vec{x},x_0;\vec{x}',x_0') = \tfrac{1}{2}\left\{-\,i\,\frac{\delta G_c(x,x')}{\delta F(\vec{x}'',\vec{x}'';x_0)} \pm i\,\frac{\delta G_c(\vec{x}'',x_0;\vec{x}',x_0')}{\delta F(\vec{x}'',\vec{x};x_0)} + G_c(x,x')\,\Psi(\vec{x}'',\vec{x}'';x_0) \mp G_c(\vec{x}'',x_0;\vec{x}',x_0')\,\Psi(\vec{x}'',\vec{x};x_0)\right\} . \qquad (8.22a)$$

The upper (lower) sign refers here to fermions (bosons). We then get from (7.7a)

$$\{i\frac{\partial}{\partial x_0} + \mu - T_{\vec{x}} - V(\vec{x})\}\, G_c(x,x') + \int d^3\vec{x}''\, F(\vec{x},\vec{x}'';x_0)\, G_c(\vec{x}'',x_0;\vec{x}',x_0') - \tfrac{1}{2}\int d^3\vec{x}''\, U(\vec{x}-\vec{x}'') \Big\{ -i\frac{\delta G_c(x,x')}{\delta F(\vec{x}'',\vec{x}'';x_0)} \pm i\frac{\delta G_c(\vec{x}'',x_0;\vec{x}',x_0')}{\delta F(\vec{x}'',\vec{x};x_0)} + G_c(x,x')\,\Psi(\vec{x}'',\vec{x}'';x_0) \mp G_c(\vec{x}'',x_0;\vec{x}',x_0')\,\Psi(\vec{x}'',\vec{x};x_0)\Big\} = -\delta(x-x')\,. \tag{8.23a}$$

Here, we have, of course,

$$G_c(x,x') = \lim_{F\to 0} G_c(x,x';F)\,, \tag{8.24a}$$

$$\Psi(\vec{x}'',\vec{x};x_0) \xrightarrow[F\to 0]{} \rho_1(\vec{x}'',\vec{x};x_0)\,. \tag{8.25}$$

9. THE MASS AND POLARISATION OPERATORS; THE EFFECTIVE WAVE EQUATION

It is often convenient for specific calculations to eliminate explicitly the functional derivative of G with respect to J by introducing some new quantities. To do this we introduce a change in the functional argument and consider G_c, R_c, ... as functionals not of J, but of $\tilde{\Phi}$.

Let us first of all consider (8.8). Clearly, we have

$$\frac{\delta G_c(x,x')}{\delta J(z)} = \int dz'\, \frac{\delta G_c(x,x')}{\delta \tilde{\Phi}(z')}\,\frac{\delta \tilde{\Phi}(z')}{\delta J(z)}\,. \tag{9.1}$$

Furthermore, we introduce the reciprocal Green function $G_c^{-1}(x,x')$, defining it by the obvious relation

$$\int G_c(x,x'')\, G_c^{-1}(x'',x')\, dx'' = \delta(x-x')\,. \tag{9.2}$$

Taking the variation of (9.2) with respect to $\tilde{\Phi}(z')$, we get

$$\int \frac{\delta G_c(x,x'')}{\delta \tilde{\Phi}(z')}\, G_c^{-1}(x'',x')\, dx'' = -\int G_c(x,x'')\,\frac{\delta G_c^{-1}(x'',x')}{\delta \tilde{\Phi}(z')}\, dx''\,,$$

whence

$$\frac{\delta G_c(x,x')}{\delta \tilde{\Phi}(z')} = -\int dy'\, dy''\, G_c(x,y')\,\frac{\delta G_c^{-1}(y',y'')}{\delta \tilde{\Phi}(z')}\, G_c(y'',x')\,.$$

We can accordingly use (8.16) to rewrite the last term on the left-hand side of (8.8) in the form

$$-ig^2\,\Gamma^{(0)}\int dy'\, dy''\, dz\; G_c(x,y')\,\frac{\delta G_c^{-1}(y',y'')}{\delta g\tilde{\Phi}(z)}\, D_c'(z,x)\; G_c(y'',x')\,. \tag{9.3}$$

We introduce the notation

$$\Gamma(x,y;z) = -\frac{\delta G_c^{-1}(x,y)}{\delta g\tilde{\Phi}(z)}, \tag{9.4}$$

$$M(x,y) = -ig^2\,\Gamma^{(0)}\int dy'\,dz\; G_c(x,y')\,\Gamma(y',y;z)\,D_c'(z,x)\,. \tag{9.5}$$

We get then instead of (9.3)

$$-\int dy''\,M(x,y'')\,G_c(y'',x')\,, \tag{9.6}$$

and instead of (8.8)

$$\{i\frac{\partial}{\partial x_0}+\mu-T_{\vec{x}}-V(\vec{x})+g\,\Gamma^{(0)}\tilde{\Phi}(x)\}\,G_c(x,x')-\int dy\,M(x,y)\,G_c(y,x') = -\delta(x-x')\,. \tag{9.7}$$

We note especially the case of a system of particles with electromagnetic interactions. Because of (6.18) we then get from (9.4), (9.5), and (9.7):

$$M(x,y) = -ig^2\,\gamma^\alpha\int du\,dv\,D_{c,\alpha\beta}'(u,x)\,G_c(x,v)\,\Gamma^\beta(v,y;u)\,, \tag{9.5a}$$

$$\Gamma^\beta(x,y;z) = -\frac{\delta G_c(x,y)}{\delta e\tilde{A}_\beta(z)} \tag{9.4a}$$

$$\{i\frac{\partial}{\partial x_0}+\mu-T_{\vec{x}}-V(\vec{x})+e\,\gamma^\beta\tilde{A}_\beta(x)\}\,G_c(x,x')-\int dy\,M(x,y)\,G_c(y,x') = -\delta(x-x')\,. \tag{9.7a}$$

Let us, moreover, consider the special case where there is no interaction with the quantum field ($g \to 0$). We get then from (9.7)

$$\{i\frac{\partial}{\partial x_0}+\mu-T_{\vec{x}}-V(\vec{x})\}\,G_c^{(0)}(x,x') = -\delta(x-x')\,. \tag{9.7b}$$

One verifies easily that when $V(\vec{x}) = 0$ (free particles and no external field) the function (5.20), indeed, satisfies this equation. Using (9.7b) we can rewrite (9.7) conveniently in a symbolic form, considering x and x' as continuous matrix arguments:

$$[G_c^{(0)}]^{-1}\,G_c - g\,\Gamma^{(0)}\,\tilde{\Phi}\,G_c + M\,G_c = 1\,. \tag{9.7c}$$

One can transform the equation for the single-boson Green function completely analogously. Let us consider an equation such as (8.10) for $D_c'(x,x')$

$$L(x)\,D_c'(x,x';J) - ig\,f\,\mathrm{Tr}\,\Gamma^{(0)}\,\frac{\delta G_c(x,x;J)}{\delta J(x')} = f\,\delta(x-x')\,, \tag{9.8}$$

where L and f are the operators introduced in section 7. By analogy with (9.1) to (9.3) we write

$$i g f \operatorname{Tr} \Gamma^{(o)} \frac{\delta G_c(x,x;J)}{\delta J(x')}$$
$$= i g^2 f \operatorname{Tr} \Gamma^{(o)} \int dy' dy'' dz\, G_c(x,y') \frac{\delta G_c^{-1}(y',y'')}{\delta g\tilde{\Phi}(z)} G_c(y'',x) D_c(z,x') \quad (9.9)$$

Using the definition (9.4) we now introduce

$$\mathcal{P}(x,y) = -i g^2 \operatorname{Tr} \Gamma^{(o)} \int dy' dy''\, G_c(x,y') \Gamma(y',y'';y)\, G_c(y'',x) . \quad (9.10)$$

The right-hand side of (9.9) then becomes

$$\int dy\, \mathcal{P}(x,y)\, D_c'(y,x') , \quad (9.11)$$

and instead of (9.8) we get

$$L(x)\, D_c'(x,x') - f \int dy\, \mathcal{P}(x,y)\, D_c'(y,x') = f\, \delta(x-x') . \quad (9.12)$$

One obtains a similar equation for Δ_c'. In the special case where there is no interaction between the quantised field and the particles ($g \to 0$) we get then

$$L(x)\, \Delta_c^{(o)}(x,x') = \delta(x-x') . \quad (9.12a)$$

We can use this equation as in the single-fermion Green function case to rewrite (9.12) into a symbolical form:

$$[\Delta_c'^{(o)}]^{-1}\, \Delta_c' - \mathcal{P}\, \Delta_c' = 1 . \quad (9.12b)$$

Let us especially consider the single-photon Green function. Using (9.10) and (6.18) we get

$$\mathcal{P}_\alpha{}^\beta(x,y) = -i e^2 g_{\alpha\delta} \operatorname{Tr} \gamma^\delta \int du\, dv\, G_c(x,u) \Gamma^\beta(u,v;y) G_c(v,x) . \quad (9.13)$$

We then get from (9.12)

$$\left(\frac{1}{c^2}\frac{\partial^2}{\partial x_o^2} - \nabla_{\vec{x}}^2\right) D_{c,\alpha\beta}'(x,x') - \int dy\, \mathcal{P}_\alpha{}^\gamma(x,y)\, D_{c,\gamma\beta}'(y,x') = g_{\alpha\beta}\, \delta(x-x') . \quad (9.14)$$

We note, in particular, the spatially uniform case when

$$D_{c,\alpha\beta}'(x,x') = D_{c,\alpha\beta}(x,x')$$
$$= \int d^3\vec{k}\, d\omega\, D_{c,\alpha\beta}(\vec{k},\omega)\, e^{-i\omega(x_o-x_o')+i(\vec{k}.\vec{x}-\vec{x}')} ,$$

$$\mathcal{P}_\alpha{}^\gamma(x,y) = \int d^3\vec{k}\, d\omega\, \mathcal{P}_\alpha{}^\gamma(\vec{k},\omega)\, e^{-i\omega(x_o-x_o')+i(\vec{k}.\vec{x}-\vec{x}')} .$$

Substituting these expansions into (9.14) we find ($k_o = \omega/c$)

$$(-k_0^2 + \vec{k}^2)\, D_{c,\alpha\beta}(k) - g^{\gamma\mu}(2\pi)^4\, \mathcal{P}_{\alpha\mu}(k)\, D_{c,\gamma\beta}(k) = \frac{g_{\alpha\beta}}{(2\pi)^4}. \quad (9.14a)$$

We note that if we use the gauge (5.35) for the function $D_{c,\alpha\beta}(k)$, we can write $\mathcal{P}_{\alpha\beta}(k)$ also in the same form:

$$\mathcal{P}_{\alpha\beta}(k) = (g_{\alpha\beta} - \frac{k_\alpha k_\beta}{k^2})\, \mathcal{P}(k)\,. \quad (9.15)$$

Indeed, because of (5.35) a term such as $k_\alpha k_\beta \mathcal{P}$ does not contribute to the product $\mathcal{P}_\alpha{}^\gamma D_{c,\gamma\beta}$.

Of course, this way of writing the equations - without further reservations - is suitable only when we evaluate gauge-invariant quantities. On the other hand, if we wish to evaluate an expression such as $\mathcal{P}_{\alpha\beta}\hat{A}^\beta$ we can use (9.15) only if the potential satisfies the Lorentz condition.

The quantities M and $\mathcal{P}$ are called, respectively, the mass and the polarisation operator. This terminology is borrowed from quantum field theory and is connected with the fact that $M(x,y)$ describes the correction to the energy (mass) of a particle when one takes into account the interaction with the quantum field (in the theory of elementary particles: with the vacuum), while $\mathcal{P}(x,y)$ takes the vacuum polarisation into account. We shall see that in electrodynamical problems the tensor $\mathcal{P}(x,y)$ indeed describes the polarisation of the medium in the most direct meaning of the word.

The function $\Gamma(x, y; z)$ is called the complete vertex part. When the interaction is vanishingly small it tends to $\Gamma^{(0)}$. Indeed, let us multiply (9.7) from the right with $G_c^{-1}(x',x'')$ and integrate over x', using (9.2). Neglecting quantities of order g^2 we get

$$\{i\frac{\partial}{\partial x_0} + \mu - T_{\vec{x}} - V(\vec{x})\}\, \delta(x-x'') + g\, \Gamma^{(0)}\, \tilde{\varphi}(x)\, \delta(x-x'') = -\, G_c^{-1}(x,x'')\,,$$

whence, using (9.4), we get

$$\Gamma(x,y;z) = \Gamma^{(0)}\, \delta(x-y)\, \delta(x-z) + O(g^2)\,. \quad (9.16)$$

Equations such as (9.7) and (9.12) were first obtained by Schwinger (1951a, b) for the case of quantum electrodynamics. Together with the supplementary Lorentz condition they are equivalent to the usual set of Maxwell and Dirac (or Schrödinger) equations. Similar equations involving functional derivatives can also be obtained for higher order Green functions (see appendix V).

Using the results of section 5 and (9.7) and (9.12) it turns out to be possible to state the problem of evaluating the energy spectrum of a system formally as a "single-particle" eigenvalue problem (Bonch-Bruevich 1959a). We assume that the potentials $V(x)$ and $\tilde{\varphi}(x)$ do not explicitly depend on the time, while the function $M(x,y)$ depends merely on a difference of time coordinates

$$M(x,y) = M(\vec{x}, \vec{y}; x_0 - y_0) \ .$$

This assumption is nothing but the necessary condition that the problem be stationary (or quasi-stationary). One can clearly only in that case talk about an energy spectrum.

In accordance with sections 4 and 5 we introduce Fourier transforms:

$$G_c(x,y) = \int_{-\infty}^{+\infty} dE \ e^{-iE(x_0 - y_0)} \ G_c(\vec{x}, \vec{y}; E) \ ,$$

$$M(x,y) = \int_{-\infty}^{+\infty} dE \ e^{-iE(x_0 - y_0)} \ M(\vec{x}, \vec{y}; E) \ .$$

We get then from (9.7)

$$\{E + \mu - T_{\vec{x}} - V(\vec{x}) + g \ \Gamma^{(0)} \ \tilde{\varphi}(x)\} \ G_c(\vec{x}, \vec{y}'; E)$$

$$- 2\pi \int d^3\vec{y} \ M(\vec{x}, \vec{y}; E) \ G_c(\vec{y}, \vec{x}'; E) = \frac{1}{2\pi} \ \delta(\vec{x} - \vec{x}') \ . \quad (9.17)$$

It is convenient to write this equation symbolically in the form

$$(E - R) \ G_c = - \frac{1}{2\pi} \ , \quad (9.17a)$$

where R is an operator defined by the left-hand side of (9.17) (it may be called the "effective Hamiltonian"). From this it follows that the poles of $G_c(\vec{x}, \vec{x}'; E)$ are the eigenvalues of the operator R. The evaluation of the spectrum is in this case thus reduced to solving the homogeneous equation

$$\{E - R(E)\} \ \chi = 0 \ , \quad (9.18)$$

where $\chi(\vec{x}, E)$ is an auxiliary function. This is the "effective wave equation"; a particular case of this is, for instance, the well-known Dirac equation with radiative corrections (Schwinger 1951a, b; Bogolyubov and Shirkov 1957).

One can formulate completely analogously the problem of finding the eigenvalues for the poles of the single-boson Green function.

Indeed, let us put

$$\Delta'_c(x,y) = \int_{-\infty}^{+\infty} dE \ e^{-iE(x_0 - y_0)} \ \Delta'_c(\vec{x}, \vec{y}; E) \ ,$$

$$\mathcal{P}(x,y) = \int_{-\infty}^{+\infty} dE \ e^{-iE(x_0 - y_0)} \ \mathcal{P}(\vec{x}, \vec{y}; E) \ .$$

We get then in complete analogy with (9.17)

$$\{- E^2 + L(\vec{x})\} \ \Delta'_c(\vec{x}, \vec{x}'; E) - 2\pi \int d^3y \ \mathcal{P}(\vec{x}, \vec{y}; E) \ \Delta'_c(\vec{y}, \vec{x}'; E)$$

$$= \frac{1}{2\pi} \ \delta(\vec{x} - \vec{x}') \ ,$$

and the poles of $\Delta'_c(\vec{x}, \vec{x}'; E)$ are thus determined from the eigenvalue problem

$$\{-E^2 + L(\vec{x})\}\, \varphi(\vec{x}, E) - 2\pi \int d^3\vec{y}\ \mathcal{P}(\vec{x}, \vec{y}; E)\, \varphi(\vec{y}, E) = 0\ . \quad (9.19)$$

Here $\varphi(\vec{x}, E)$ is an auxiliary function.

It is important to note that the special properties of the G_c and Δ'_c are nowhere used in the derivation of (9.18) and (9.19). Effective wave equations of this kind are thus valid (under the above-mentioned conditions) for any double-time quantities of the kind (3.17). In all these cases we get for the determination of the corresponding branch of the spectrum of a system of N interacting particles, generally speaking, an equation in an r-dimensional space, where r is the number of independent variables occurring in the set λ. Only the explicit form of the operators such as $R(E)$ depends then on the specific nature of the operators C_1 and C_2 in (3.17).

Equations such as (9.18) and (9.19) give apparently the most obvious basis for the concept of a gas of quasi-particles with a temperature-dependent spectrum.

We must, however, emphasise that in practice this concept is justified, inasfar as it is at all justified, by the spectral theorems of sections 4 and 5. The only advantage of equations such as (9.18) and (9.19) is their great translucency.

We must make a few remarks in connexion with what has been said so far.

First of all, we obtained (9.18) - and similar equations - without making any assumptions about the interaction being small, about series expansions, and so on, and its interpretation is based solely upon the spectral properties of the Green functions, that is, upon exact relations. Moreover, after we have established a connexion between the energy spectrum of a system and the spectral properties of the Green functions (section 5) the possibility of introducing in an exact manner such "single-particle", "two-particle", ... equations becomes nearly trivial.

Secondly, eigenvalue problems such as (9.18) are as a rule non-Hermitean. The diagonal elements of the mass, the polarisation, and other similar operators may, for instance, have finite imaginary parts. As a result the eigenvalues E may turn out to be complex (there is damping). One must thus consider together with (9.18), (9.19), ... also their complex conjugates.

Thirdly, equations such as (9.18) only appear as single-particle equations; in actual fact, the interaction effects are completely taken into account in them. This manifests itself in the fact that these equations can not, strictly speaking, been considered independently. For instance, the single-boson Green function occurs in the definition of the mass operator. This difficulty is sometimes circumvented in actual problems by semi-phenomenological means (see section 24).

Fourthly, effective wave equations are, as a rule, non-linear: the mass and polarisation operators depend on G_c and D'_c.

Fifthly and finally, (9.18) and similar equations differ from the usual eigenvalue problems in that the parameter E occurs non-linearly: the operator R depends itself on E through $M(\vec{x}, \vec{y}; E)$.

These last two facts make it impossible to express in the usual way $G_c(\vec{x}, \vec{y}; E)$, $\Delta'_c(\vec{x}, \vec{y}; E)$, ... in terms of the solutions of (9.18), (9.19) and the complex conjugate equations.

One general deduction can be made from (9.18) and (9.19). We saw in chapter I that the frequencies E which determine the singularities of the Green functions are independent of the volume V of the system *. The operators on the left-hand sides of the effective wave equations are thus also independent of the volume, that is, both the mass and the polarisation operator are volume-independent in the limit as $V \to \infty$. It follows thus that the volume of the system does not occur in the equations for the Green functions, asymptotically as $V \to \infty$, that is, the Green functions are not extensive, but intensive quantities.

If $G \sim \delta(\lambda - \lambda')$, as happens, for instance, in the momentum representation in a uniform system, what we have said refers to the coefficient of the δ-functions.

Let us now consider the particular case where the Fourier transform of the mass (or polarisation, ...) operator $M(\vec{x}, \vec{y}; E)$ (i) is independent of E, that is, $M(x, y)$ contains a factor $\delta(x_0 - y_0)$, (ii) is given a priori, that is, does not contain the Green function we wish to find, and (iii) is Hermitean. Of course, such a situation can, at any rate for the simplest Green functions, occur only approximately. This occurs, for instance, in systems with instantaneous (in particular, Coulomb) interactions, if we assume these to be sufficiently weak and restrict ourselves to the first non-vanishing approximation in the coupling constant (see section 11).

Under these conditions (9.18) becomes a standard linear Hermitean eigenvalue problem and the Green function can be expressed as the usual bilinear expansion in terms of the $\chi(\vec{x}, E)$. This has then a direct physical meaning which we elucidate by finding the connexion between χ and the Green functions. Indeed, let us denote by u the set of parameters which distinguish the eigenfunctions χ and let us put

$$G_c(\vec{x}, \vec{x}'; E) = -\frac{1}{2\pi} \int du\ \chi(\vec{x}, u)\ \chi^+(\vec{x}', u) \left\{ \frac{a(u)}{E - E(u) - i\varepsilon} + \frac{b(u)}{E - E(u) + i\varepsilon} \right\} \tag{9.20}$$

(the integral may, as always, include a sum, if (9.18) possesses a discrete spectrum). Using the completeness condition

* We are here, of course, only referring to the asymptotic properties valid as $V \to \infty$. Until this limiting process has been carried out the energy spectrum can, of course, depend on the dimensions of the system.

$$\int du\ \chi(\vec{x},u)\ \chi^{+}(\vec{x}',u) = \delta(\vec{x}-\vec{x}')\ ,$$

we see that the right-hand side of (9.20) satisfies (9.17), provided

$$a(u) + b(u) = 1\ . \tag{9.21}$$

The ratio a/b is determined by the boundary conditions imposed upon $G_c(\vec{x},\vec{x}';E)$. We mentioned in sections 6 and 7 that these conditions may be replaced by the dispersion relations of section 4. In the present case, where we are dealing with the causal function, we must use (4.10):

$$\operatorname{Re} G_c(\vec{x},\vec{x};E) = \frac{1}{\pi}\int_{-\infty}^{+\infty} dE'\,\frac{1+e^{-\beta E'}}{1-e^{-\beta E'}}\,\mathcal{P}\,\frac{\operatorname{Im} G_c(\vec{x},\vec{x};E')}{E'-E}\ .$$

It is convenient to change variables in (9.20) and to choose as one of the parameters u the energy $E(u) \equiv E$; we denote the rest of the parameters collectively by v, and the Jacobian of the transformation from u to (E',v) by $Z(E',v)$. We get then

$$G_c(\vec{x},\vec{x}';E) = -\frac{1}{2\pi}\int_{-\infty}^{+\infty} dE' \int dv\ Z(E',v)\ \chi(\vec{x},E',v)\ \chi^{+}(\vec{x}',E',v)$$

$$\times\left\{\frac{a(E',v)}{E-E'-i\varepsilon}+\frac{b(E',v)}{E-E'+i\varepsilon}\right\}\ . \tag{9.22}$$

We note that in actual cases the integral over E' is, generally speaking, not from $-\infty$ to $+\infty$, but naturally between the lower and the upper bounds of the spectrum. Indeed, $\chi(\vec{x},E',v) \equiv 0$, unless E' is an eigenvalue of (9.18). Because of this we shall in the following drop the limits on the integrals.

We assume that a and b are real and depend only on the energy (this will be justified by our calculations: we shall see that we can in this way, indeed, satisfy the boundary conditions). We get then by putting $\vec{x}' = \vec{x}$ in (9.22) and separating the real and the imaginary parts

$$\operatorname{Im} G_c(\vec{x},\vec{x};E) = -\frac{a-b}{2}\int |\chi(\vec{x},E,v)|^2\ Z(E,v)\,dv\ , \tag{9.23}$$

$$\operatorname{Re} G_c(\vec{x},\vec{x};E) = -\frac{1}{\pi}\int dE'\,\mathcal{P}\,\frac{\operatorname{Im} G_c(\vec{x},\vec{x};E')}{E'-E}\cdot\frac{a+b}{a-b}\ . \tag{9.24}$$

From (4.10) we then get

$$\frac{a+b}{a-b} = -\frac{1+e^{-\beta E'}}{1-e^{-\beta E'}}\ .$$

Combining this with (9.21) we get

$$a(E') = \frac{1}{1+e^{\beta E'}} \equiv n_F(E')\ , \qquad b(E') = \frac{1}{1+e^{-\beta E'}} \equiv 1 - n_F(E')\ . \tag{9.25}$$

We have thus

$$G_c(\vec{x},\vec{x}';E) = -\frac{1}{2\pi}\int dE'\,dv\; Z(E',v)\;\chi(\vec{x},E',v)\;\chi^+(\vec{x}',E',v) \times\left\{\frac{n_F(E')}{E-E'-i\varepsilon}+\frac{1-n_F(E')}{E-E'+i\varepsilon}\right\}. \tag{9.26}$$

We can do exactly the same for the functions $G^{(+)}_{r,a}$. One sees easily that (9.26) is formally the same as the Green function of a system of independent fermions which satisfy a wave function with Hamiltonian R (compare (5.13) and (5.14)). The sum over λ is now replaced by an integral over v with a weight function $Z(E',v)$. This is an important argument in favour of the expediency of our determination of a temperature-dependent spectrum. We note here that because of (5.4) we have (N: total number of particles in the system)

$$i\int d^3\vec{x}\,\mathrm{Tr}\lim_{\substack{x'\to x\\ x'_0>x_0}} G_c(x,x') = i\int d^3\vec{x}\lim_{\substack{t\to 0\\ t<0}}\int_{-\infty}^{+\infty} dE\; e^{-iEt}\mathrm{Tr}\; G_c(\vec{x},\vec{x};E) = N,$$

and thus, using (9.26)

$$\int dE\;dv\;Z(E,v)\;n_F(E)\int d^3(\vec{x})\;|\chi(\vec{x},E,v)|^2 = N\,. \tag{9.27}$$

If the function χ has a continuous spectrum, the integral of $|\chi|^2$ over $\vec{x}$ will be proportional to V as $V\to\infty$. It is, however, convenient to normalise χ:

$$\mathrm{Tr}\int d^3x\;\;|\chi(\vec{x},E,v)|^2 = 1\,. \tag{9.28}$$

To do this we divide the integral over $\vec{x}$ by V, simultaneously introducing a factor V in Z. In the following we shall thus assume that

$$Z(E,v) = V\,Z'(E,v)\,, \tag{9.29}$$

where the function Z' is asymptotically (as $V\to\infty$) independent of V.

Comparing (9.23) and (9.25) with (4.9) we can find the spectral function J for the product of two fermion operators a and a^+ (we remind ourselves that we do not write down explicitly the spin indices assuming J and G_c to be spin matrices). We get

$$J(\vec{x},E) = \frac{\int dv\;|\chi(\vec{x},E,v)|^2}{1+e^{-\beta E}}\,, \tag{9.30}$$

and accordingly the matrix elements of the single-particle density matrix (1.9) connected with fermion-operators are of the form

$$(\vec{x}\,|\rho_1|\,\vec{x}')_F = \int_{-\infty}^{+\infty} dE\int dv\,\frac{Z(E,v)}{1+e^{\beta E}}\chi(\vec{x},E,v)\;\chi^+(\vec{x}',E,v)\,. \tag{9.31}$$

As we could have expected because of (9.26), (9.31) is formally the same as the matrix element of the operator ρ_1 for a system of independent fermions with wave functions $\chi(\vec{x},E,v)$ and energies E. In that sense $\chi(\vec{x},E,v)$ can be called the "effective wave function"; we must emphasise, however, that it can only be used to evaluate averages of additive dynamical variables.

In the same way we get for a system of bosons

$$G_c(\vec{x},\vec{x}';E) = \frac{1}{2\pi}\int dE'\,dv\; Z(E',v)\;\chi(\vec{x},E',v)\;\chi^+(\vec{x}',E',v) \times\left\{\frac{n_B(E')}{E-E'-i\varepsilon} - \frac{1+n_B(E')}{E-E'+i\varepsilon}\right\}, \tag{9.32}$$

where

$$n_B(E') = \frac{1}{e^{\beta E'}-1}.$$

One can accordingly write the matrix elements of the operator ρ_1 in the form

$$(\vec{x}\,|\,\rho_1\,|\,\vec{x}')_B = \int dE\,dv\,\frac{Z(E,v)}{e^{\beta E}-1}\,\chi(\vec{x},E,v)\;\chi^+(\vec{x}',E,v)\,. \tag{9.33}$$

One must, however, bear in mind that (9,31) and (9.33) define, generally speaking, only part of the matrix elements of the operator (1.9). Indeed, in (1.9) there occur operators a and a^+ of all possible types, among them field operators (provided we are dealing with a system of particles which interact with a quantised field). The matrix ρ_1 must thus contain apart from the "corpuscular" part (9.31) also a "field" part. We can easily find it like (9.31) and (9.33) under the above mentioned conditions by writing down the bilinear expansion similar to (9.20) for the appropriate Green function. We note here that the quantity E^2 plays in fact in (9.19) the role of the eigenvalue. As before, we denote by u the parameters which number the eigenfunctions $\varphi(\vec{x})$, and we change from u to the variables (E^2,v). By complete analogy with (9.22) we get

$$\Delta_c(\vec{x},\vec{x}';E^2) = -\frac{1}{2\pi}\int dE'^2\,dv\; Z(E'^2,v)\;\varphi(\vec{x},E'^2,v)\;\varphi^+(\vec{x}',E'^2,v) \times\left\{\frac{a}{E^2-E'^2-i\varepsilon}+\frac{b}{E^2-E'^2+i\varepsilon}\right\}, \tag{9.34}$$

where the functions a and b must satisfy (9.21). Comparing (9.34) with the dispersion relation (5.32) (written down for Δ_c) we find

$$\frac{a+b}{a-b} = -\frac{1-e^{-\beta E}}{1+e^{-\beta E}},$$

and hence, using (9.21)

$$a = -n_B\,, \qquad b = 1+n_B\,. \tag{9.35}$$

Thus

$$\Delta_c(\vec{x}, \vec{x}'; E^2) = \frac{1}{2\pi} \int dE'^2\, dv\, Z(E'^2, v)\, \varphi(\vec{x}, E'^2, v) \cdot \varphi^+(\vec{x}', E'^2, v) \times \left\{ \frac{n_B}{E^2 - E'^2 - i\varepsilon} - \frac{1 + n_B}{E^2 - E'^2 + i\varepsilon} \right\} \tag{9.36}$$

(one verifies easily that the expression within the braces in (9.36) depends, indeed, only on E'^2).

We can also write down an effective wave equation such as (9.19) for the function F_c of (7.26), and repeating word for word all previous discussions we can obtain an expression such as (9.34) (moreover with the same spectrum). In fact, the spectral function for F_c can also be used to express the "field" part of the single-particle density matrix. One can also easily verify that (9.26) and (9.31) to (9.34) are valid also if we replace $\vec{x}$ by arbitrary dynamical variables λ.

One can also define in a natural way the mass operator for a system of particles with direct interactions (see Klein and Prange 1958a, Kogan 1960). In fact, we write by definition

$$\int d\lambda_1\, d\lambda_2\, d\lambda_3\, (\lambda, \lambda_1 | U | \lambda_3, \lambda_2)\, G_{2,c}(\lambda_1, \lambda_2, \lambda_3; x_0; \lambda', x_0') = \int d\lambda_1\, dx_0''\, M(\lambda, x_0; \lambda_1, x_0'')\, G_c(\lambda_1, x_0''; \lambda', x_0') \,. \tag{9.37}$$

In particular, (9.37) is in the coordinate representation (see (7.7a))

$$\int d^3\vec{x}''\, U(\vec{x} - \vec{x}'')\, G_{2,c}(\vec{x}'', \vec{x}'', \vec{x}, x_0; \vec{x}', x_0') = \int dx''\, M(x, x'')\, G_c(x'', x') \,. \tag{9.37a}$$

Using (9.37) we can write

$$M(\lambda, x_0; \lambda', x_0') = \int d\lambda_1\, d\lambda_2\, d\lambda_3\, d\lambda_4\, dx_0''(\lambda_1, \lambda_2 | U | \lambda_3, \lambda_2) \times G_{2,c}(\lambda_1, \lambda_2, \lambda_3, x_0; \lambda_4, x_0'')\, G_c^{-1}(\lambda_4, x_0''; \lambda', x_0'). \tag{9.38}$$

It is sometimes convenient to write this formula in four-dimensional form, putting

$$(x, x_1 | U | x_3, x_2) = \delta(x_0 - x_{0,1})\, \delta(x_0 - x_{0,2})\, \delta(x_0 - x_{0,3})\, (\lambda, \lambda_1 | U | \lambda_3, \lambda_2) \,. \tag{9.39}$$

We have then

$$M(x, x') = \int d^4x_1\, d^4x_2\, d^4x_3\, d^4x_4 (x, x_1 | U | x_3, x_2) \times G_{2,c}(x_2, x_3; x_1, x_4)\, G_c^{-1}(x_4, x') \,, \tag{9.40}$$

where $G_{2,c}(x_2, x_3; x_1, x_4) = i <T\{a(x_2)a(x_3)a^+(x_1)a^+(x_4)\}>$ (9.41)

is the two-particle Green function in the general form.

After we introduce the mass operator, (7.7) is formally changed into an integro-differential equation for $G_c(x,x')$; in actual fact, however, it is necessary when evaluating $M(x,x')$ to "decouple" the chain (7.7) in some way or other *.

The equation for the Fourier transform $G_c(\vec{x}, \vec{x}'; E)$ can then be written in a form similar to (9.17):

$$\{E - R(\vec{x}, E)\} G_c(\vec{x}, \vec{x}'; E) = -\frac{1}{2\pi} \delta(\vec{x}-\vec{x}') , \qquad (9.42)$$

where the operator R is defined by the equation

$$R(\vec{x}, E)\, G_c(\vec{x}, \vec{x}'; E) = \{T_{\vec{x}} + V(\vec{x}) - \mu\}\, G_c(\vec{x}, \vec{x}'; E) + 2\pi \int d^3\vec{x}''\, M(\vec{x}, \vec{x}''; E)\, G_c(\vec{x}'', \vec{x}'; E) . \qquad (9.43)$$

It is clear that in that case we can also introduce an effective wave equation such as (9.18) with all consequences following from this. In particular, under the above-mentioned conditions we have the bilinear expansion (9.26) and (9.31).

One can also write down expansions such as (9.26) and (9.34) for higher-order double-time Green functions, provided the conditions of Hermiticeity and linearity of the appropriate effective wave equations are satisfied. The functions χ and φ will then, however, generally speaking, depend on a larger number of arguments and will satisfy symmetry or antisymmetry conditions with respect to the interchange of two arguments. In the following we need a bilinear expansion for the function (5.24):

$$G_{2,c}(t) = i <T\{a^+(\vec{x}_1, x_0)a(\vec{x}_2, x_0)a^+(\vec{x}_1', x_0')a(\vec{x}_2', x_0')\}> .$$

The appropriate dispersion relation for this function is (4.10) with $\eta = 1$, and the bilinear expansion has thus exactly the boson form (compare (9.32))

$$G_{2,c}(E) = \frac{1}{2\pi} \int dE'\, dv\, Z_2(E', v)\, \chi_2(\vec{x}_1, \vec{x}_2, E', v)\, \chi_2^+(x_1', x_2', E', v) \times \left\{ \frac{n_B(E')}{E - E' - i\varepsilon} - \frac{1 + n_B(E')}{E - E' + i\varepsilon} \right\} . \qquad (9.44)$$

The index "2" of Z and χ reminds us of the fact that we are dealing with functions connected with the effective wave equation for $G_{2,c}(\vec{x}, \vec{x}'; E)$.

* For details see appendix VI.

10. DYSON'S EQUATIONS AND THE MULTIPLICATIVE RENORMALISATION GROUP

Equations (9.7) and (9.12) are differential equations because of the occurrence of the operators $T_{\vec{x}}$ and $L(x)$. They can in the usual manner be transformed into integral equations by introducing into the discussion the Green functions $G_c^{(0)}$ and $D_c^{(0)}$ (the solutions of (9.7b) and (9.12a)) of the free fields. To do this we only need to consider terms which contain the coupling constant g formally as being the inhomogeneous term and use the normal properties of Green functions as source functions. We get in this way from (9.7) and (9.12)

$$G_c(x,x') = G_c^{(0)}(x,x') + g\int dx''\, G_c^{(0)}(x,x'')\,\Gamma^{(0)}\,\tilde{\Phi}(x'')\,G_c(x'',x') - \int dz\,dz'\,G_c^{(0)}(x,z)\,M(z,z')\,G_c(z',x')\,, \tag{10.1}$$

$$D_c'(x,x') = D_c'^{(0)}(x,x') + \int du\,dv\,D_c'^{(0)}(x,u)\,\mathcal{P}(u,v)\,D_c'(v,x')\,, \tag{10.2}$$

or, symbolically

$$G_c = G_c^{(0)} + g\,G_c^{(0)}\,\Gamma^{(0)}\,\tilde{\Phi}\,G_c - G_c^{(0)}\,M\,G_c\,, \tag{10.1a}$$

$$D_c' = D_c'^{(0)} + D_c'^{(0)}\,\mathcal{P}\,D_c'\,. \tag{10.2a}$$

From (10.2a) especially it can clearly be seen what is the meaning of replacing the boundary conditions (understood in the literal sense) by dispersion relations such as (4.7), (4.8), or (4.10). Indeed, formally we get from (10.2a)

$$D_c' = \frac{1}{[D_c'^{(0)}]^{-1} - \mathcal{P}}\,. \tag{10.2b}$$

In practice, however, this expression taken as it stands has no meaning, if the eigenvalues of the denominator can vanish. It becomes well defined, if we state how to go around the poles. This reduces, however, to writing down a well-defined connexion between the real and the imaginary parts of D_c', that is, dispersion relations.

In a similar way we can write down an equation for the average potential (8.12). We get, symbolically,

$$\tilde{A}_\alpha = -\,D_{c,\alpha\beta}'^{(0)}\,(J^\beta + i\,e\,g^{\beta\mu}\,\mathrm{Tr}\,\gamma_\mu\,G_c)\,. \tag{10.3}$$

This formula is a special case of the easily obtained general equation of motion for the potential, $\tilde{\Phi}$

$$\tilde{\Phi} = -\,D_c'^{(0)}\,(J + i\,g\,\Gamma^{(0)}\,G_c). \tag{10.3a}$$

We must add to this equation the definitions of the mass and the polarisation operator, (9.5) and (9.10). These are symbolically of the form

$$M = -ig^2\,\Gamma^{(0)}\,G_c\,\Gamma\,D'_c\,, \tag{10.4}$$

$$\mathcal{P} = -ig^2\,\mathrm{Tr}\,\Gamma^{(0)}\,G_c\,\Gamma\,G_c\,. \tag{10.5}$$

Equations (10.1) to (10.5) are called Dyson's equations. One usually employs these for the actual determination of the causal Green functions.

We emphasise once again that G_c and D'_c (and hence $G_c^{(0)}$ and $D_c'^{(0)}$) must satisfy the boundary conditions (3.21) or the dispersion relation (4.10) which is their equivalent. (We are, of course, dealing here, as in section 9, with boundary conditions with respect to the variable $t = x_0 - x'_0$.) One can formulate the condition (3.21) as a condition of periodicity in the "imaginary temperature", and accordingly one can expand the functions we are looking for in Fourier series (Martin and Schwinger 1959, Fradkin 1959a, b). It is more convenient for us to use directly the dispersion relations (a similar method is used in quantum field theory; Bogolyubov, Logunov, and Shirkov 1959). This enables us to expand the function we are looking for in a Fourier integral (and not a Fourier series) in the frequency. We did this, for instance, in section 9 when constructing the Green functions from the solutions of the effective wave equation. It is sometimes sufficient to determine the imaginary part of the appropriate Green function from Dyson's equations and then to find its real part directly from the dispersion relations. We note in this connexion that we saw in section 4 that we need to know just the imaginary part of the Green functions to evaluate the spectral functions and all characteristics of the system connected with them. It thus turns out to be possible in some approximate calculations to manage completely without the real parts of the Green functions.

Dyson's equations possess one important property which we shall use in the following for an essential improvement of approximate calculations in the framework of perturbation theory. One verifies, namely, easily directly that these equations are invariant under the multiplicative transformations

$$G_c \to z_2\,G_c\,, \quad D'_c \to z_3\,D'_c\,, \quad \Gamma \to z_1^{-1}\,\Gamma\,, \quad \tilde{\Phi} \to z_3^{\frac{1}{2}}\,\tilde{\Phi}\,, \tag{10.6}$$

$$g^2 \to z_2^{-2}\,z_3^{-1}\,z_1^2\,g^2\,, \tag{10.7}$$

where z_1, z_2, and z_3 are finite, continuous parameters (see Blank, Bonch-Bruevich, and Shirkov 1957). We have assumed here that the transformation is applied not only to the "complete" functions G_c, D'_c, and Γ, but also to the "unperturbed" ones, $G_c^{(0)}$, $D_c'^{(0)}$, and $\Gamma^{(0)}$.

It is clear that the transformations (10.6), (10.7) form a group

(the so-called renormalisation group) *. We note that they can be appreciably simplified, if there are some additional conditions (in that case the parameters z_1, z_2, and z_3 may not be independent). For instance, when there are forces of electromagnetic nature present an important relation follows from the condition of gauge invariance. Indeed, it is well known from quantum mechanics that when the potentials are gauge-transformed according to (5.33) the wave function in the coordinate representation is multiplied by

$$\exp\left[\frac{i}{c}\sum_a e_a f(x_a)\right], \tag{10.8}$$

where a numbers the particles in the system, and e_a is the charge of the a-th particle. Because of (10.6) the function f transforms as $f \to z_3^{1/2} f$. On the other hand, (10.8) must be invariant under the transformations of the renormalisation group (the gauge-invariance can not depend on the choice of the parameters z_1, z_2, and z_3). The electrical charge must thus transform as follows

$$e^2 \to z_3^{-1} e^2, \tag{10.9}$$

that is, for a system with electromagnetic (in particular, Coulomb) interactions we have the identity

$$z_1 = z_2 . \tag{10.10}$$

This relation is called Ward's identity (1950).

Because of (10.10) we get instead of (10.6) and (10.7) for a system with electromagnetic interactions the simpler relations

$$\begin{gathered} G_c \to z\, G_c , \quad D_c' \to z_3\, D_c', \quad \Gamma \to z^{-1}\, \Gamma , \\ e^2 \to z_3^{-1}\, e^2 , \quad \tilde{A} \to z_3^{1/2}\, \tilde{A} . \end{gathered} \tag{10.11}$$

We emphasise that (10.11) is also valid for a system of neutral particles if their interactions are caused by the superposition of electrical fields.

* The renormalisation group was first discovered in connexion with quantum field theory problems. Its name is connected with the fact that originally the parameters z_1, z_2, and z_3 played the role of the (in general infinite) renormalisation constants occurring when one removed explicitly the divergences from the scattering matrix (Dyson 1949). It became clear only later that even after the infinities had been removed Dyson's equations admitted the multiplicative group (10.6), (10.7) with finite parameters z_1, z_2, and z_3 (Stueckelberg and Petermann 1953, Bogolyubov and Shirkov 1955). Finally, Blank, Bonch-Bruevich, and Shirkov (1957) shewed that this fact is not at all connected with the presence of divergencies and is not peculiar for relativistic quantum field theory, but is a general property of the Dyson equations for a very broad class of interaction Hamiltonians.

11. IMPROVED PERTURBATION THEORY

The solution of (10.1) and (10.2) is a problem of exceptional complexity, and there are as of the present no general "prescriptions". In the present section we shall give a very simple approximate method to evaluate Green functions (Bonch-Bruevich 1956a, 1957a) which is based upon expanding the mass and polarisation operators in power series in the coupling constant with a subsequent improvement in convergence by using the renormalisation group. (We assume that we have used such a system of units that the coupling constant g is dimensionless.) We emphasise from the beginning that this method has only a limited region of applicability - even if the coupling constant is sufficiently small - as it excludes from our considerations cases where the dependence on g is non-analytical as g tends to zero (superconductivity theory is the most important example of a problem of that type). At the same time a large number of problems (in particular, those connected with the Coulomb interactions between electrons in a solid) can be completely treated in this way.

We shall restrict ourselves to the case of a spatially uniform system which is of most interest to us in the following. Performing a Fourier transform, we get from (10.1) and (10.2)

$$G_c(p) = \frac{G_c^{(0)}(p)}{1 + (2\pi)^8 G_c^{(0)}(p) M(p)}, \tag{11.1}$$

$$D_c(k) = \frac{D_c^{(0)}(k)}{1 - (2\pi)^8 D_c^{(0)}(k) \mathcal{P}(k)}. \tag{11.2}$$

The rule for going around the poles in (11.1) and (11.2) is derived from the dispersion relations according to the discussion of the preceding section.

Let us compare (11.2) (applied to a system of charged particles with electromagnetic interactions) with (8.17). From this comparison it is at once clear that the expression $1 - (2\pi)^8 D_c^{(0)}(k) \mathcal{P}(k)$ has the physical meaning of a generalised dielectrical constant (which depends on frequency and wave vector), and this justifies the terminology "polarisation operator".

Equations (11.1) and (11.2) are exact non-linear integral equations for G_c and D_c. We shall solve them, evaluating $M(p)$ and $\mathcal{P}(k)$ by iteration. We shall call this a perturbation theory method. One must, however, bear in mind that this is in actual fact a more subtle method than the standard perturbation method used, for instance, to evaluate the S-matrix (see appendix I). We do not expand the Green functions G_c and D_c themselves in powers of the coupling constant, but their denominators, that is the reciprocal functions G_c^{-1} and D_c^{-1}. This is very important. It is clear from the results of section 5 that

possible changes in the energy spectrum connected with the presence of interactions are reflected in the poles of G_c and D_c. If we consider a power series expansion of G_c^{-1} and D_c^{-1} we only allow the well-known shift in the determination of the spectrum to occur; on the other hand, power series expansions of the Green functions themselves would lead to a complete "loss" of the influence of interactions upon the spectrum of the system: the poles of G_c and D_c remain in that case the same as those of $G_c^{(0)}$ and $D_c^{(0)}$.

One can state this somewhat differently. A power series expansion of $M(k)$ and $\mathcal{P}(k)$ under well-defined conditions may have a meaning in the whole of momentum space; it is, however, immediately clear from (11.1) and (11.2) that an expansion of the functions $G_c(p)$ and $D_c(k)$ themselves may turn out to be without any meaning in the regions near the poles of the "free" functions $G_c^{(0)}(p)$ and $D_c^{(0)}(k)$.

From (9.5), (9.10), and (9.16) we get in the first non-vanishing approximation in the coupling constant *

$$M(p) \cong M^{(0)}(p) = -\,i g^2 \int dp'\; \Gamma^{(0)}\, G_c^{(0)}(p')\, \Gamma^{(0)}\, D_c^{(0)}(p'-p)\,, \qquad (11.3)$$

$$\mathcal{P}(k) \cong \mathcal{P}^{(0)}(k) = -\,i g^2\, \mathrm{Tr} \int dk'\; \Gamma^{(0)}\, G_c^{(0)}(k')\, \Gamma^{(0)}\, G_c^{(0)}(k'-k)\,. \qquad (11.4)$$

The meaning of the approximation (11.3) becomes especially clear if we use the effective wave equation (9.18) and restrict ourselves for the sake of simplicity to the case $\Gamma^{(0)} = 1$ and $D_c^{(0)}(p) = D_c^{(0)}(\vec{p})$ (this is the case when we have a non-relativistic system with instantaneous interactions, in particular in the case of Coulomb interactions in a solid; compare (5.39)). The mass operator (11.3) becomes under these conditions

$$\begin{aligned} M^{(0)}(p) &= -\,i g^2 \int d^3\vec{p}'\, D_c^{(0)}(\vec{p}'-\vec{p}) \int_{-\infty}^{+\infty} dp_0'\, G_c^{(0)}(p') \\ &= -\,g^2 \int d^3\vec{p}'\, D_c^{(0)}(\vec{p}'-\vec{p})\, n_0(\vec{p}') = M^{(0)}(\vec{p}) \in \mathrm{Re}\,. \end{aligned} \qquad (11.5)$$

Here, $n_0(\vec{p}')$ is the average occupation number for the state $\vec{p}'$ when there are no interactions (using (5.5)). The last term in the quantity $R\,\chi$ (in the momentum-representation) will then be

$$-\,(2\pi)^4 g^2 \int d^3\vec{p}'\, D_c^{(0)}(\vec{p}'-\vec{p})\, n_0(\vec{p}')\, \chi(\vec{p})\,. \qquad (11.5a)$$

We note that we would have obtained the same formally if we had substituted for G_c into (11.3) not $G_c^{(0)}$, but expression (9.26). We would then have had instead of $n_0(\vec{p})$, $2\,|\chi(\vec{p})|^2$ (the factor 2 arises from the trace over the spin variable) and (9.18) would become of the form

* We note that in quantum electrodynamics the approximation (11.4) gives at once the results obtained by Landau, Abrikosov, and Khalatnikov (1954).

typical for the self-consistent field method; the only differences with the usual Hartree equation would be (i) a non-vanishing temperature, and (ii) a potential which involves screening. The form (9.26) for $G_C(\vec{x}, \vec{x}'; E)$ with D_C replaced by $D_C^{(0)}$ in the mass operator is thus equivalent to the Hartree approximation (generalised to a finite temperature); the approximation (11.3) with $n_0(\vec{p}')$ in (11.5a) assumed to be given is the linearised Hartree method.

The substitution of (11.3) and (11.4) into (11.1) and (11.2) solves in the present approximation the problem of determining the causal Green functions; moreover, we can use (4.9) to find the corresponding spectral functions.

To find the next approximation we need only substitute into the mass and the polarisation operator the functions G_C, D_C, ..., which we have found. We note that in general we do not in this case obtain consistent expansions in terms of the coupling constant but "mixed-up" expressions in which the coupling constant may occur only in a power series, but also in a more complicated manner (see the example in section 23).

We must emphasise that in general one can not find the limits of applicability of the expressions obtained in this way by formally estimating the magnitude of the dimensionless constant g. First of all, the actual expansion parameter may turn out to be (and in fact does turn out to be) different in different regions of momentum space *. Secondly, in the statistical problem - especially at finite temperatures - there are usually several dimensionless quantities, and the condition that the corrections from the next approximation are small involves inequalities which as a rule contain all these parameters. To estimate the magnitude of the actual expansion parameter it is clearly most convenient to use the method of the renormalisation group, and we shall do this here, applying it to the isotropic case. The basic idea is to perform the expansion such as (11.3) or (11.4) only in a small region of momentum space, and then extend the results to the whole of momentum space using the group equations (10.6) and (10.7). We shall see that these equations reduce to differential equations and we thus must give their boundary conditions. To do this we try to determine a priori the behaviour of $D_C(k)$ in some region of momentum space. In the following we restrict ourselves only to systems with instantaneous interactions and forces of electromagnetic origin (this means: either systems of charged particles interacting through Coulomb forces, or systems of neutral atoms or molecules). Using (5.39) and (8.17) we see that in that case $D_C^{(0)}(k)$ depends on $\vec{k}$ only; the possibility of D_C depending on k_0 is due to "radiative corrections". We can thus only know the form of $D_C(\vec{k}, k_0)$ a priori for $k_0 = 0$ (of course, in a range of $\vec{k}$-values).

* This fact is well known in quantum field theory (Bogolyubov and Shirkov 1957, Landau, Abrikosov, and Khalatnikov 1954).

To do this we rewrite (8.17), introducing in it the Fourier transform $D'_c(x, x')$. We remind ourselves of the fact that in the case considered here of a spatially uniform system the functions D'_c and D_c are the same. (We have, of course, in view a system which is spatially uniform when there are no external fields.) We shall assume here that $J(x')$ is independent of x'_0 (static "charge"). We get then

$$\tilde{\varphi}(\vec{x}) = (2\pi)^4 \int d^3\vec{k}\, D_c(\vec{k}, k_0)\Big|_{k_0=0} e^{i(\vec{k}.\vec{x})}\, J(\vec{k}) , \qquad (11.6)$$

where

$$J(\vec{k}) = \frac{1}{(2\pi)^3} \int d^3\vec{x}\, e^{-i(\vec{k}.\vec{x})}\, J(\vec{x}) . \qquad (11.7)$$

In particular when we have a point source at $\vec{x} = 0$, $J(\vec{x}) = I_m\, \delta(\vec{x})$ (I_m: constant) and

$$\tilde{\varphi}(\vec{x}) = 2\pi I_m \int d^3\vec{k}\, D_c(\vec{k}, k_0)\Big|_{k_0=0} e^{i(\vec{k}.\vec{x})} . \qquad (11.8)$$

From this it is clear that the difference between $D_c(\vec{k}, 0)$ and $D_c^{(0)}(\vec{k})$ indicates nothing but the "screening" of the external field by the particles in the system (compare the discussion following (11.2)). It is clear that this effect can not occur at sufficiently small distances from the sources of the field. The form of $\tilde{\varphi}(\vec{x})$ at small $|\vec{x}|$ is, however, determined by the behaviour of $D_c(\vec{k}, 0)$ for large $|\vec{k}|$. We must thus have the following limit:

$$D_c(k) \xrightarrow[\substack{k_0 = 0 \\ |\vec{k}| \to \infty}} D_c^{(0)}(\vec{k}) . \qquad (11.9)$$

We shall use this equation as the boundary condition for solving the renormalisation group equations. These have for the present case the form (10.11):

$$G_c \to z\, G_c , \quad \Gamma \to z^{-1}\, \Gamma , \quad D_c \to z_3\, D_c , \quad g^2 \to z_3^{-1}\, g^2 . \qquad (11.10)$$

We must thus first of all study the behaviour of D_c as the "charge" g^2 is connected with it.

We put

$$D_c(k) = D_c^{(0)}(k)\, d(k) , \qquad (11.11)$$

where $D_c^{(0)}(k)$ is an explicitly given known function, and $d(k)$ the new unknown for which we also shall write down the group equation. As the function $d(k)$ is dimensionless by definition (the dimensions of D_c and $D_c^{(0)}$ are the same), it can depend only on the ratio of dimensional variables; moreover, as it is scalar, it must be explicitly expressed in terms of scalar combinations of its arguments. We shall choose a system of units where the mass is dimensionless (and, as always, where $\hbar = 1$). We denote by W_0 all independent characteristic energies which determine the properties of the system (for instance, this

would be for a metal the Fermi energy, for a semiconductor kT, and, perhaps a parameter such as $n^{2/3}/2m_0$, and so on). Because of (11.10) D_c, G_c, and Γ contain an arbitrary (continuously varying) parameter. This enables us to introduce a (so far undetermined) "normalisation energy" λ, putting

$$d(k) = d(\frac{\omega}{\lambda}, \frac{k^2}{\lambda}, \frac{W_0}{\lambda}; g^2) . \tag{11.12}$$

We note that just at this point the assumption about the uniformity of the system crops up. In the anisotropic case (which can occur in the electron theory of solids) we have instead of one independent scalar $\vec{k}^2$ two, namely, $\vec{k}^2$ and $W(\vec{k})$, where $W(\vec{k})$ is the energy of an electron as function of its quasi-momentum. The calculations are then somewhat more complicated, although not essentially different.

As the boundary condition (11.9) is imposed at $\omega = 0$, we shall first of all consider that case. We introduce the notation

$$d(\vec{k}, \omega)\Big|_{\omega=0} = d_0(\frac{\vec{k}^2}{\lambda}, \frac{W_0}{\lambda}; g^2) . \tag{11.13}$$

Equation (11.10) shews that we may multiply d by an arbitrary constant, provided we change g^2 accordingly. We can thus normalise d_0:

$$d_0(1, \frac{W_0}{\lambda}; g^2) = 1 . \tag{11.14}$$

This means that when $\vec{k}^2 = \lambda$ the function $D_c(\vec{k}, 0)$ is the same as $D_c^{(0)}(\vec{k})$: there are no "radiative corrections". One must, however, remember that a transformation of d entails a transformation of the coupling constant g; for arbitrary λ we can therefore not have for g in (11.14) the present "charge". The true ("real") charge g is obtained from (11.14) only, if that equation agrees with the boundary condition (11.9). This reduces to a well-defined choice of λ: the true value of g corresponds to $\lambda \to \infty$.

We shall establish here a functional and differential equation for $d_0(\vec{k}^2/\lambda, W_0/\lambda; g^2)$. We denote by λ_1 and λ_2 two different values of the normalisation energy and by g_1 and g_2 the corresponding coupling constants. From (11.10) and (11.14) we get

$$d_0(\frac{\vec{k}^2}{\lambda_1}, \frac{W_0}{\lambda_1}; g_1^2) = z_3\, d_0(\frac{\vec{k}^2}{\lambda_2}, \frac{W_0}{\lambda_2}; g_2^2) ,$$

$$g_2^2 = z_3 g_1^2 , \qquad z_3 = d_0(\frac{\lambda_2}{\lambda_1}, \frac{W_0}{\lambda_1}; g_1^2) .$$

For the sake of simplicity we put

$$\lambda_1 \equiv \lambda , \quad g_1 \equiv g , \quad \frac{\vec{k}^2}{\lambda_1} = u , \quad \frac{W_0}{\lambda_1} = v , \quad \frac{\lambda_2}{\lambda_1} = w . \tag{11.15}$$

We get then

$$d_0(u,v;g^2) = d_0(w,v;g^2)\, d_0(\tfrac{u}{w}\,,\ \tfrac{v}{w}\,;\ g^2\, d_0(w,v;g^2)) \ . \qquad (11.16)$$

This is the functional equation of the renormalisation group.

One must, however, bear in mind that this equation is insufficient, even in conjunction with (11.14) and (11.9), to determine $d_0(u,v;g^2)$ uniquely: one can shew (Ovsyannikov 1956) that the general solution of (11.16) contains an arbitrary function of two arguments. As in field theory (Bogolyubov and Shirkov 1957) we impose the additional condition that the answer should correspond with the perturbation theory answer in the limit of vanishingly small coupling constants. It is convenient in this connexion to change (11.16) into a differential equation. Differentiating (11.16) with respect to u and after that putting $w = u$, we get

$$\frac{\partial}{\partial u}\, g^2\, d_0(u,v;g^2) = \frac{g^2\, d_0(u,v;g^2)}{u}\, [\frac{\mathrm{d}}{\mathrm{d}\xi}\, d_0(\xi,\ \frac{v}{u};\ g^2\, d_0(u,v;g^2))]_{\xi=1} \ . \qquad (11.17)$$

Equation (11.17) is nothing but one of the Lee equations describing the renormalisation group (11.10). The boundary condition for (11.17) follows from (11.14) and (11.9). As W_0 is finite, it is

$$d_0(u,v;g^2) \underset{\substack{u\to 1\\ v\to 0}}{\longrightarrow} 1 \ . \qquad (11.18)$$

The derivative with respect to ξ occurring on the right-hand side of (11.17) will be defined using the perturbation theory developed earlier (and this guarantees then the agreement with perturbation theory as $g \to 0$). In this connexion we must draw attention to two important facts. Firstly, we use here perturbation theory not to find d_0 in the whole of momentum space, but only in an infinitesimal neighbourhood of the "normalisation point" $\xi = 1$. In particular, this does not enable us to avoid the above mentioned difficulty with the poles. Secondly, and even more importantly, the expansion parameter is here not the coupling constant g^2 itself, but the quantity

$$g^2_{\mathrm{inv}} = g^2\, d_0(u,v;g^2) \ . \qquad (11.19)$$

We shall call expression (11.19) the "invariant charge" as it is invariant under the renormalisation group transformations of (11.10). It is clear that the invariant charge is different in different regions of momentum space, and that this is the way to define the true expansion parameter.

We note that the quantity g^2_{inv} of (11.19) has an immediate physical meaning: from a comparison with (11.8) it is clear that it is the "screened" coupling constant, attenuated because all the interactions of the particles in the medium are taken into account. We can thus

say that the main meaning of the renormalisation group lies in the fact that the quantities we are looking for are expanded in terms of the screened and not the "true" charge (it is clear from physical considerations that the latter is always larger than the former; this can be verified by direct calculations).

In the first non-vanishing perturbation theory approximation d_0 is given by (11.2) with the polarisation operator (11.4) (with $\omega = 0$). Since the product $\mathcal{P}^{(0)}(k)\, D_c^{(0)}(k)$ is dimensionless, it can depend only on the ratio of its arguments:

$$(2\pi)^8\, \mathcal{P}^{(0)}(k)\, D_c^{(0)}(k)\Big|_{\omega=0} = g^2 f\left(\frac{k^2}{W_0}\right) \equiv g^2 f\left(\frac{u}{v}\right) \qquad (11.20)$$

(the precise form of f is, of course, different for different cases). We get thus, neglecting higher order terms and taking the normalisation (11.14) into account,

$$d_0\left(\xi, \frac{v}{u}; g^2\, d_0(u,v;g^2)\right) \cong 1 + g^2\, d_0(u,v;g^2)\, \left\{f\left(\frac{\xi u}{v}\right) - f\left(\frac{u}{v}\right)\right\} . \qquad (11.21)$$

Substituting this into (11.17) and using the boundary condition (11.18) we find easily

$$d_0(u,v;g^2) = \frac{1}{1 - g^2 f\left(\frac{u}{v}\right)} . \qquad (11.22)$$

This formula can be applied provided

$$\frac{g^2}{1 - g^2 f\left(\frac{u}{v}\right)} \ll 1 . \qquad (11.23)$$

We shall see in the following that in a number of cases $f(u/v) < 0$ and the inequality (11.23) may be much weaker than $g^2 \ll 1$.

We now turn to the determination of $d(k)$ when $\omega \neq 0$. We put

$$d(k) = S^{-1}(t,u,v;g^2) , \qquad (11.24)$$

where

$$t = \frac{\omega + k^2}{\lambda} , \qquad (11.25)$$

while u and v are given by (11.25). We have clearly

$$S(u,u,v;g^2) = d_0^{-1}(u,v;g^2) \quad (= 1 \text{ when } u = 1) . \qquad (11.26)$$

The differential equation for S is easily obtained by the method described earlier:

$$\frac{\partial S(t,u,v;g^2)}{\partial t} = \frac{d_0^{-1}(t,v;g^2)}{t}\left[\frac{\mathrm{d}}{\mathrm{d}\xi} S\left(\xi, \frac{u}{t}, \frac{v}{t}; g^2\, d_0(t,v;g^2)\right)\right]_{\xi=1} . \qquad (11.27)$$

The boundary condition of (11.27) is (11.26). From dimensional considerations we get

$$(2\pi)^8\ \mathcal{P}(o)(k)\ D_c^{(o)}(k) = g^2\ \varphi(\frac{t}{v}, \frac{u}{v})\ . \qquad (11.28)$$

Clearly, we have $\varphi(u/v, u/v) = f(u/v)$. When we evaluate the derivative in (11.27) we use again, as before, perturbation theory assuming the following inequality to be satisfied:

$$g^2\ d_o(t, v; g^2) \ll 1\ . \qquad (11.29)$$

Using (11.26), we then get from (11.27)

$$S(t, u, v; g^2) \cong 1 - g^2\ \varphi(\frac{t}{v}, \frac{u}{v})\ . \qquad (11.30)$$

We see thus that if (11.23) and (11.29) are satisfied, the expression obtained from perturbation theory for $D_c(k)$ is valid (both for $\omega = 0$ and for $\omega \neq 0$); its applicability does, however, not reduce to the trivial requirement $g^2 \ll 1$. It is especially important that in general it does not follow from (11.29) that $g^2\ \varphi(t/v, u/v)$ is small. This quality may well be comparable with unity under these conditions, and this fact enables us in principle to study by the method developed here the occurrence of new poles in the Green functions.

We can use a completely analogous method to evaluate $G_c(p)$. We put

$$G_c(p) = G_c^{(o)}(p)\ Q^{-1}(p)\ .$$

Using (11.10), (11.15), and (11.25) we get the following functional equation for Q:

$$Q(t, u, v; g^2) = \frac{Q(w, w, v; g^2)\ Q(\frac{t}{w}, \frac{u}{w}, \frac{v}{w}; g^2\ d_o(w, v; g^2))}{Q(1, 1, \frac{v}{w}; g^2\ d_o(w, v; g^2))}\ . \qquad (11.31)$$

The function Q depends on two variables t and u, and in this case it is analogous to the vertex part in quantum electrodynamics. One can easily use for (11.31) the methods developed in connexion with the quantum electrodynamics case (Blank and Shirkov 1956); we do not need these, however, in the following.

For systems with direct interactions we can also develop a perturbation theory similar to the one discussed above *. The first approximation consists then in replacing the two-particle Green function in (7.7) by its value for $H_{int} = 0$:

$$G_{2,c}(\lambda', \lambda'', \lambda''', x_o; \lambda_1, x_o') = i\ G_c(\lambda'', x_o; \lambda', x_o)\ G\ (\lambda''', x_o; \lambda_1, x_o')$$

$$- i\ G_c(\lambda''', x_o; \lambda', x_o)\ G\ (\lambda'', x_o; \lambda_1, x_o')\ . \qquad (11.32)$$

* One can also easily develop perturbation theory in a functional form by introducing, completely as in section 9, a mass operator and a vertex part. All the same, however, it is necessary to decouple the equation for the two-particle Green function (see appendix VI).

The Green functions with equal arguments are defined using (5.5).

Using (9.40) we then get for the mass operator for a system with pair interactions

$$M(x,x') = 2\,\mathrm{i}\int \mathrm{d}x_1\,\mathrm{d}x_2 (x,x_1|U|x',x_2)\,G_c(x_2,x_1)\,. \qquad (11.33)$$

This equation is valid both for fermion and for boson systems. We remind ourselves that the matrix $(x,x_1|U|x',x_2)$ is either antisymmetric or symmetric with respect to the interchanges $x \to x_1$ and $x' \to x_2$, and that the arguments λ_1, λ_2, ... include also the spin variables.

The approximation (11.33) is, however, not suitable for system having potentials such as hard-sphere potentials. It is also not very satisfactory for systems with regular, but strong interactions.

In the case where the interaction forces are non-vanishing only at sufficiently small distances (of the order of some characteristic length a), it turns out to be possible to develop a special form of perturbation theory (Galitskiĭ 1958, Belyaev 1958b) where the role of the small expansion parameter is played neither by the invariant charge (11.19) nor by the "coupling constant", but by the product $a\,n^{1/3}$ (where n is the particle concentration and a a small, though finite quantity). We try, namely, to express the mass operator in terms of the scattering amplitude of the particles (which retains its meaning also for singular potentials) and not in terms of the interaction potential. Because of our assumption that the parameter $an^{1/3}$ be small, it is then sufficient to consider only the case where the particles are scattered in the vacuum. In other words, in each well-defined stage of the calculations we neglect the "screened" action of the complete system of particles and take only the pair-wise collisions between them into account.

Bearing this transition to the scattering amplitude in mind we introduce a new operator Q by putting

$$M(x,x') = \int \mathrm{d}x_1\,\mathrm{d}x_2 (x,x_1|Q|x',x_2)\,G_c(x_2,x_1)\,. \qquad (11.34)$$

(We assume that the matrix elements $(x,x_1|Q|x',x_2)$ satisfy the necessary symmetry requirements, determined by the statistics of the particles in the system.)

We obtain the equation for Q by comparing (11.34) with the definition (9.37) of the mass operator. We restrict ourselves to the case of spatially uniform systems. It is then convenient to us the momentum representation, putting $\lambda = \{p,s\}$, where s is the spin coordinate, We have then clearly

$$G_c(\lambda,x_0;\lambda',x_0) = \delta(p-p')\,G_c(p;s,s')\,,$$

and

$$(\lambda,x_0,\lambda_1,x_{1,0}|U|\lambda',x_0',\lambda_2,x_{2,0}) = \delta(p_1+p-p'-p_2)\,U'(p,s,p_1,s_1;p',s',p_2,s_2)\,. \qquad (11.35)$$

We can similarly introduce quantities Q' and $G'_{2,c}$. Comparing (11.34) and (9.37), we find easily

$$\int dp'\, Q'(p,s,p',s_1;p,s',p',s_2)\, G_c(p';s_1,s_2)$$
$$= G_c^{-1}(p;s_4,s') \int d^4p'\, d^4p''\, d^4p'''\, \delta(p+p'-p''-p''')$$
$$U'(p,s,p',s_1;p'',s_2,p''',s_3)\, G'_{2,c}(p'',s_3,p''',s_2;p',s_1,p,s_4) \qquad (11.36)$$

(we assume summation over spin indices occurring twice).

We shall restrict ourselves in the following to spin-independent forces. We then have

$$G_c(p;s,s') = \delta_{ss'}\, G_c(p)\ ;$$

$$Q'(p,s,p',s_1;p'',s_2,p''',s_3) = \delta_{ss_2}\, \delta_{s_1s_3}\, Q'(p,p';p''',p'') \qquad (11.37)$$
$$\pm\, \delta_{ss_3}\, \delta_{s_1s_2}\, Q'(p,p';p'',p''')\ .$$

The upper (+) sign refers to bosons and the lower (-) sign to fermions. One should no longer impose on the Q' on the right-hand side of (11.37) the antisymmetry (or symmetry) condition. One can also write $G'_{2,c}$ and U' in the same form (it is clearly sufficient to assume only one of them, say U, to be antisymmetrised, as only their product enters into (11.36)). We get thus for the mass operator (S is the spin of one particle)

$$M_1(p_1;s,s') = -(2\pi)^8\, \delta_{ss'}\, \{(2S+1) \int d^4p\, G_c(p)\, Q'(p_1,p;p_1,p)$$
$$\pm \int dp\, G_c(p)\, Q'(p_1,p;p,p_1)\}\ , \qquad (11.38)$$

and (11.36) becomes

$$\int dp\, G_c(p)\, Q'(p_1,p;p_1,p) = \int d^4p_2\, d^4p_3\, d^4p_4\, \delta(p_1+p_2-p_3-p_4)$$
$$\times\, U'(p_1,p_2;p_3,p_4)\, G_c^{-1}(p_1)\, G'_{2,c}(p_4,p_3;p_2,p_1)\ , \qquad (11.39)$$

$$U'(p_1,p_2;p_3,p_4) = \frac{1}{(2\pi)^{12}} \int d^4x\, U(x)\, e^{-ikx}\Big|_{k=\frac{1}{2}(p_1-p_2-p_3+p_4)} \qquad (11.40)$$

(it is clearly sufficient to write down this equation for only one of the terms in (11.37)). We put furthermore

$$Q'(p_1,p_2;p_3,p_4) = \int d^4q\, U(q)\, S(p_1-q,p_2+q;p_3,p_4)\ . \qquad (11.41)$$

Substituting this into (11.39) we see that we can choose for S the expression

$$S(p_1,p_2;p_3,p_4) = \frac{1}{(2\pi)^8}\, G_c^{-1}(p_3)\; G_c^{-1}(p_4)\; G'_{2,c}(p_1, p_2; p_4, p_3)\ . \quad (11.42)$$

We must here satisfy the relation

$$p_1 + p_2 - p_3 - p_4 = 0\ . \quad (11.43)$$

Using (11.42) we get immediately the equation for S from the equation for the two-particle Green function $G_{2,c}$. This last equation is derived in appendix V. Using the fact that the parameter $an^{1/3}$ is supposed to be small we can limit ourselves to the approximate formulae (V.11) and (V.12). Changing over to the Fourier transform in (V.11) and using (11.35) and (11.37) (for $G_{2,c}$) we get

$$G_c^{-1}(p_1)\; G_c^{-1}(p_2)\; G'_{2,c}(p_1,p_2;p_3,p_4)$$

$$- (2\pi)^8\, i \int d^4p\; U(p)\; G'_{2,c}(p_1-p, p_2+p; p_3, p_4) = - i\, \delta(p_1-p_4)\ , \quad (11.44)$$

where the momenta p_1, p_2, p_3, and p_4 satisfy (11.43). Combining (11.44) and (11.42), and using (11.43), we get

$$S(p_1, p_2; p_3, p_4) - i\,(2\pi)^8 \int d^4q\; U(q)\; G_c(p_1)\; G_c(p_2)\; S(p_1-q, p_2+q; p_3, p_4)$$

$$= - i\, \delta(p_1-p_3)\ . \quad (11.45)$$

It is convenient to introduce new variables, putting

$$p_1+p_2 = p_3+p_4 = p\ ; \qquad p_1-p_2 = 2\,k'; \qquad p_3-p_4 = 2k''\ . \quad (11.46)$$

It is clear that p is the four-momentum of the centre of mass of the system of two-particles (which is conserved during a collision), and k' and k'' are the relative momenta before and after the collision. In these variables we can write (11.45) in the form

$$S(k', k''; p) - i\,(2\pi)^8\; G_c\left(\frac{p}{2}+k'\right)\; G_c\left(\frac{p}{2}-k'\right) \int d^4q\; U(q)\; S(k'-q, k''; p)$$

$$= - i\, \delta(k'-k'')\ . \quad (11.47)$$

We now change to the variables (11.46) in the right-hand side of (11.41). We then get

$$Q'(k', k''; p) = \int d^4q\; U(q)\, S(k'-q, k''; p)\ . \quad (11.48)$$

Since the interaction is not retarded (that is, $U(x)$ contains a factor $\delta(x_0)$), we have $U(q) = U(\vec{q})$, that is, $U(q)$ is independent of q_0. From this it is clear that it is sufficient to evaluate instead of S itself its integral over the fourth momentum component

$$F(\vec{k}', \vec{k}''; p) = \int dk'_0\; S(k', k''; p)\ . \quad (11.49)$$

Integrating (11.47) over k'_0, we get

$$F(\vec{k}', \vec{k}''; p) - J \int d^3\vec{q}\; U(\vec{q})\, F(\vec{k}' - \vec{q}, \vec{k}''; p) = - i\, \delta(\vec{k}' - \vec{k}'') , \quad (11.50)$$

where

$$J = i\,(2\pi)^8 \int dk'_0\, G_c(\frac{p}{2} + k')\; G_c(\frac{p}{2} - k') .$$

In the present approximation we must substitute for G_c the Green function $G_{c,vac}$ for a single particle in the vacuum. One verifies easily that this function is given by the expression

$$G_{c,vac}(p) = - \frac{1}{(2\pi)^4} \cdot \frac{1}{p_0 - \vec{p}^2/2m + i\epsilon} , \quad (11.51)$$

and thus

$$J = \frac{2\pi}{p_0 - \dfrac{p^2}{4m} - \dfrac{\vec{k}'^2}{m} + i\eta} .$$

We get thus from (11.50)

$$F(\vec{k}', \vec{k}''; p) - \frac{2\pi}{E - \dfrac{\vec{k}'^2}{m} + i\eta} \int d^3\vec{q}\; U(\vec{q})\; F(\vec{k}' - \vec{q}, \vec{k}''; p) = - i\, \delta(\vec{k}' - \vec{k}'') , \quad (11.52)$$

where $E = p_0 - (p^2/4m)$.

The corresponding homogeneous equation is formally nothing but the equation for the relative motion of two particles, in momentum representation. One must remember that m is here the mass of one particle and that thus the reduced mass is $m/2$. We shall assume that we know the solution of the homogeneous equation (or rather, some of its integrals: vide infra), and we shall denote it by $\chi^{\pm}_{\vec{k}}(\vec{k}')$, where $\vec{k}$ is the relative momentum at infinity. Using the relation

$$\int d^3\vec{k}\; \chi^{\pm}_{\vec{k}}(\vec{k}')\; \chi^{\mp}_{\vec{k}}(\vec{k}'') = \delta(\vec{k}' - \vec{k}'') ,$$

we find easily

$$F(\vec{k}', \vec{k}''; p) = - i \int d^3\vec{k}\; \frac{E - \dfrac{\vec{k}''^2}{m} + i\eta}{E - \dfrac{\vec{k}^2}{m} + i\eta}\; \chi^{-}_{\vec{k}}(\vec{k}')\; \chi^{+}_{\vec{k}}(\vec{k}'') . \quad (11.53)$$

Using (11.48) and (11.49) we now get

$$Q'(\vec{k}', \vec{k}''; p) = - i \int d^3\vec{q}\; d^3\vec{k}\; U(\vec{q}) \frac{E - \dfrac{\vec{k}''^2}{m} + i\eta}{E - \dfrac{\vec{k}^2}{m} + i\eta}\; \chi^{-}_{\vec{k}}(\vec{k}' - \vec{q})\; \chi^{+}_{\vec{k}}(\vec{k}'') . \quad (11.54)$$

We introduce the scattering amplitude of the particles $f(\vec{k}', \vec{k})$ by the equation

$$\chi^{+}_{\vec{k}}(\vec{k}') = \delta(\vec{k}-\vec{k}') + \frac{4\pi f(\vec{k}', \vec{k})}{\vec{k}^2 - \vec{k}'^2 + i\eta} \tag{11.55}$$

It is clear that

$$f(\vec{k}', \vec{k}) = m \int d^3\vec{q}\; U(\vec{q})\; \chi^{+}_{\vec{k}}(\vec{k}' - \vec{q}) , \tag{11.56}$$

and (11.54) can thus be written in the form

$$Q'(\vec{k}', \vec{k}''; p) = -\frac{i}{m} \int d^3\vec{k}\, \frac{E - \frac{\vec{k}''^2}{m} + i\eta}{E - \frac{\vec{k}^2}{m} + i\eta}\, \chi^{+}_{\vec{k}}(\vec{k}'') f(\vec{k}', \vec{k})$$

$$= -\frac{i}{m} \{ f(\vec{k}', \vec{k}'') + 4\pi \int d^3\vec{k}\, \frac{E - \frac{\vec{k}''^2}{m} + i\eta}{E - \frac{\vec{k}^2}{m} + i\eta} \cdot \frac{f^{+}(\vec{k}'', \vec{k}) f(\vec{k}', \vec{k})}{\vec{k}^2 - \vec{k}'^2 - i\eta} \} . \tag{11.57}$$

The function Q' we are looking for can thus be expressed directly in terms of the scattering amplitude, without involving at all explicitly the interaction potential. This enables us to develop a special form of perturbation theory in which the quantities we wish to find are expanded in power series not in the interaction energy, but in the parameter $an^{1/3}$. In particular, in the first approximation we must neglect the second term within the braces in (11.57). In other words, we can formally use here the ordinary perturbation theory, merely replacing the matrix $U'(p_1, p_2; p_1, p_2)$ by

$$\frac{1}{2m} f\left(\frac{\vec{p}_1 - \vec{p}_2}{2}, \frac{\vec{p}_1 - \vec{p}_2}{2}\right) .$$

We then get for the mass operator

$$M(p_1; s, s') = i\,(2\pi)^8\, \delta_{ss'}\, \frac{1}{m} \left\{ (2S+1) \int d^4p\; G_c(p)\, f\left(\frac{\vec{p}_1 - \vec{p}}{2}, \frac{\vec{p}_1 - \vec{p}}{2}\right) \right.$$

$$\left. \pm \int d^4p\; G_c(p)\, f\left(\frac{\vec{p}_1 - \vec{p}}{2}, \frac{\vec{p} - \vec{p}_1}{2}\right) \right\} . \tag{11.58}$$

We know (see section 5) that the integral of $G_c(\vec{p}, p_0)$ over p_0 gives us the particle momentum distribution function $n(\vec{p})$, which is normalised to the occupation number:

$$\int_{-\infty}^{+\infty} dp_0\; G_c(\vec{p}, p_0) = \pm \frac{i}{(2\pi)^3}\, n(\vec{p}) \tag{11.59}$$

(the upper (lower) sign refers to the boson (fermion) case). We get thus in this first approximation for the mass operator

$$M(p_1; s, s') = \frac{(2\pi)^5}{m}\,\delta_{ss'}\left\{\mp(2S+1)\int d^3\vec{p}\; n(\vec{p})\, f\left(\frac{\vec{p}_1-\vec{p}}{2}, \frac{\vec{p}_1-\vec{p}}{2}\right)\right.$$
$$\left. - \int d^3\vec{p}\; n(\vec{p})\, f\left(\frac{\vec{p}_1-\vec{p}}{2}, \frac{\vec{p}-\vec{p}_1}{2}\right)\right\}. \qquad (11.60)$$

In the next approximation we must take into account the difference between the Green function and its "vacuum" value (11.51); the mass operator will then in general be temperature-dependent.

Chapter III

GREEN FUNCTIONS AND THE MACROSCOPIC CHARACTERISTICS OF A SYSTEM

12. GREEN FUNCTIONS AND THE THERMODYNAMIC POTENTIAL

The connexion between the Green functions and the density matrix follows from the spectral theorems of sections 4 and 5. We saw there that once we know the s-particle Green function, we can determine the corresponding spectral function; the latter, in its turn, is the Fourier transform of the matrix element of the s-particle density matrix.

In the present section we shall give equations connecting the thermodynamic potential Ω of the system directly with the simplest Green functions: the single-, two-fermion, and the single-boson Green function, and also with the vertex part. We shall perform explicit calculations for fermion systems. Changing our results to the case of boson systems requires only a few changes of signs (and will be indicated where necessary). That one can give such a connexion is due to the specific character of the interaction energy which is either a pair interaction or an interaction through a quantum field. It is convenient to consider these two cases separately.

a. *Interactions through quantum fields* *. In accordance with what we saw in section 6, we write the Hamiltonian of the system in this case as follows:

$$H' = H'_{\mathrm{p}} + H_{\mathrm{f}} + H_{\mathrm{pf}} , \tag{12.1}$$

where in accordance with (6.17)

$$H_{\mathrm{pf}} = - g \int \mathrm{d}^3 \vec{x} \; a^+(x) \; \Gamma^{(0)} \, a(x) \; \varphi(x) \equiv g \, h . \tag{12.2}$$

The operator h does not contain the coupling constant g. The actual value of the time coordinate of the Heisenberg operators a, a^+, and φ in (12.1) and (12.2) is not important (H' is an integral of motion). In the following we shall assume it to be equal to zero for the sake of simplicity.

From (1.6) we have

$$\Omega = - \beta^{-1} \ln \mathrm{Trace} \; \mathrm{e}^{-\beta H'} . \tag{12.3}$$

* Bonch-Bruevich 1959b, Kogan 1959, 1960.

We put

$$\Omega = \Omega_0 + \Omega_{pf} , \tag{12.4}$$

where $$\Omega_0 = - \beta^{-1} \ln \mathrm{Trace}\, e^{-\beta(H_p' + H_f)} . \tag{12.5}$$

It is evident that Ω_0 is the thermodynamic potential of a system of non-interacting particles (as a rule one can easily find this quantity). Differentiating (12.3) with respect to g we get

$$\frac{\partial \Omega}{\partial g} = \langle h \rangle = \frac{1}{g} \langle H_{pf} \rangle . \tag{12.6}$$

Using the boundary condition $\Omega \xrightarrow[g \to 0]{} \Omega_0$, we find from this

$$\Omega_{pf} = \int_0^g \frac{dg'}{g'} \langle H_{pf} \rangle , \tag{12.7}$$

where the average $\langle H_{pf} \rangle$ in (12.7) must be evaluated with the coupling constant being equal to g'. As $T \to 0$ ($\beta \to \infty$) this formula gives the shift ΔE_0 in the ground state energy of the system when the interaction between the particles and the quantum field is taken into account. One must, however, draw attention to the essential difference between the expressions for ΔE_0 and Ω_{pf}. In the first case, (12.7) gives an explicit expression for ΔE_0, as $\beta \to \infty$; on the other hand, Ω_{pf} is only determined implicitly by (12.7), as the average $\langle H_{pf} \rangle$ itself depends on Ω. We note that in general the self-energy also occurs in (12.7). In some problems (for instance when studying electron-phonon interactions) this self-energy is of real physical interest and one can then use (12.7) directly. In a number of cases, however, the self-energy bears no relation to the problem considered and must be eliminated. This is, for instance, the case when we consider a system of particles interacting with electromagnetic, and in particular with Coulomb forces. We shall in the following denote this elimination of the self-energy by $[\ldots]'$.

We now substitute (12.2) for the interaction Hamiltonian into (12.7). We then get

$$\Omega_{pf} = - \int_0^g \frac{dg'}{g'} \int d^3\vec{x}\, g' \langle a^+(x)\, \Gamma^{(0)}\, a(x)\, \Phi(x) \rangle . \tag{12.8}$$

We can transform this expression in two ways.

Firstly, we write $\langle a^+(x)\, a(x)\, \Phi(x) \rangle$ in its spectral form (we display here the spin indices s and s' explicitly)

$$\langle a^+(\vec{x}, s)\, a(\vec{x}, s')\, \Phi(\vec{x}) \rangle = \int_{-\infty}^{+\infty} dE\, J(\vec{x}, s, s'; E) . \tag{12.9}$$

We then get

$$\Omega_{pf} = - \int_0^g dg' \int d^3\vec{x} \int_{-\infty}^{+\infty} dE\, \Gamma^{(0)}(s, s')\, J(\vec{x}, s, s'; E) . \tag{12.10}$$

Since the operators a^+a and Φ taken at the same time commute, the complete product $a^+a\Phi$ is Hermitean, and the integral $\int dE\, J(\vec{x},s,s';E)$ is thus real. The quantity Ω_{pf} is thus real, as it should, of course, be.

If we apply (12.8) and (12.10) to a system of charged particles (interacting through the electromagnetic field) we must take into account the condition that the system as a whole is neutral. In other words, we must take into account not only the interaction of the particles considered with one another (through the field), but also with the field of the classical sources. The corresponding Hamiltonian is

$$-\int d^3\vec{x}\; i^\beta(\vec{x})\; \tilde{A}_\beta(\vec{x})\ .$$

Here i^β is the current density four-vector; we have not denoted this here by J^β as is done in other parts of this book, in order to avoid confusion with the spectral functions. Adding this expression to the right-hand side of (12.10) and using (6.18) for $\Gamma^{(o)}$ we get

$$\Omega_{pf} = -\int_0^e de' \int d^3\vec{x}\; \{\int_{-\infty}^{+\infty} dE\; \gamma^\beta\, [J_\beta(\vec{x},E)]' + i^\beta(\vec{x})\; \tilde{A}_\beta(\vec{x})\}\ . \quad (12.11)$$

The spectral function is in the present case clearly a four-vector, J_β.

Secondly, if we wish to express Ω_{pf} in terms of the mass and polarisation operators, introduced in section 9, we write (12.8) as follows:

$$\Omega_{pf} = -\int_0^g \frac{dg'}{g'} \int d^4x\; \delta(x_o)\; g' \langle a^+(x)\; \Gamma^{(o)}\; a(x)\; \Phi(x)\rangle\ . \quad (12.12)$$

We transform the average of the triple product, using (8.4) and (9.1) to (9.6); in that way we get (explicitly displaying the trace over the spin variables)

$$g'\ \mathrm{Tr} \langle a^+(x)\; \Gamma^{(o)}\; a(x)\; \Phi(x)\rangle = -g' \lim_{\substack{x'\to x \\ x'_o > x_o}} \mathrm{Tr}\; \Gamma^{(o)} \langle T\, \{a(x)\; a^+(x')\; \Phi(x)\}\rangle$$

$$= g' \lim_{\substack{x'\to x \\ x'_o > x_o \\ i\to 0}} \mathrm{Tr}\; \Gamma^{(o)}\; \{\langle S\rangle \frac{\delta G_c(x,x')}{\delta i(x)} + i\, G_c(x,x')\; \tilde{\Phi}(x)\}$$

$$= \lim_{\substack{x'\to x \\ x'_o \to x_o}} \mathrm{Tr}\, \{-i \int d^4y\; M(x,y)\; G_c(y,x') + ig'\; \Gamma^{(o)}\; G_c(x,x')\; \tilde{\Phi}(x)\}\ . \quad (12.13)$$

We have thus

$$\Omega_{pf} = -\int_0^g \frac{dg'}{g'} \int d^4x\, \delta(x_0) \lim_{\substack{x' \to x \\ x_0 > x_0}} \mathrm{Tr}\, \{ -i \int d^4y\, M(x,y)\, G_c(y,x') + i g' \Gamma^{(0)}\, G_c(x,x')\, \tilde{\varphi}(x) \} . \quad (12.14)$$

For a system of charged particles we get by analogy with (12.11)

$$\Omega_{pf} = i \int d^4x\, d^4y \lim_{\substack{x' \to x \\ x_0 > x_0}} \int_0^e \frac{de'}{e'} \delta(x_0)\, \mathrm{Tr}\, [M(x,y)\, G_c(y,x')]'$$

$$- \int_0^e \frac{de'}{e'} \int d^4x\, \delta(x_0) \{ i e' \mathrm{Tr}\, \gamma^\beta\, G_c(x,x)\, \tilde{A}_\beta(x) + i^\mu(x)\, \tilde{A}_\mu(x) \} . \quad (12.15)$$

The expression $G_c(x,x)$ is defined by using (5.5). We note that one can easily check by using (9.5a) and (9.13) that the last term on the right-hand is exactly equal to

$$i \int d^4x\, d^4y \lim_{\substack{x' \to x \\ x_0 > x_0}} \int_0^e \frac{de'}{e'} \delta(x_0) [\mathcal{P}^{\alpha\beta}(x,y)\, D'_{c,\alpha\beta}(y,x')]' . \quad (12.15a)$$

We shall consider especially the spatially uniform case. We put, as usual

$$G_c(x,y) = \int d^4p\, G_c(p)\, e^{-i(p,x-y)} ,$$
$$M(x,y) = \int d^4p\, M(p)\, e^{-i(p,x-y)} . \quad (12.16)$$

Substituting (12.16) into (12.14) we integrate first of all over y and x_0. We get

$$\int d^4x\, d^4y\, \delta(x_0) \lim_{\substack{x' \to x \\ x'_0 > x_0}} M(x,y)\, G_c(y,x')$$
$$= (2\pi)^4 \lim_{\substack{t \to 0 \\ t<0}} \int d^4p\, M(p)\, G_c(p)\, e^{-ip_0 t} \int d^3\vec{x} .$$

The last integral gives us the volume V. The divergence as $V \to \infty$ is a completely natural one: we are evaluating the total thermodynamic potential (and not the thermodynamic potential per particle), and that is an extensive quantity. For the first terms on the right-hand sides of (12,14) and (12.15) we get thus

$$(2\pi)^4 \, \mathrm{i} \, V \int_0^g \frac{\mathrm{d}g'}{g'} \lim_{\substack{t\to 0 \\ t<0}} \mathrm{Tr} \int \mathrm{d}^4 p \, [M(p) \, G_c(p) \, \mathrm{e}^{-\mathrm{i}p_0 t}]' \, . \quad (12.17)$$

The second term in (12.15) must be dropped for a spatially uniform system with electromagnetic interactions, because of the neutrality condition. As far as other systems are concerned, there is some physical interest in either a system of electrons interacting with phonons, or an ensemble of neutral particles for which the pair interactions are described through some quantum field (see section 8). In both these cases $\Gamma^{(0)} = 1$, and the second term on the right-hand side of (12.14) is of the form

$$-\mathrm{i} \int_0^g \mathrm{d}g' \int \mathrm{d}^4 x \, \delta(x_0) \, n(\vec{x}) \, \tilde{\Phi}(x) \, , \quad (12.18)$$

where $n(\vec{x})$ is the average particle concentration at $\vec{x}$ (see (5.4)). In the case of spatially uniform systems $n(\vec{x}) = n$ = constant; moreover, when $i = 0$ we get from (10.3a) and (5.5)

$$\tilde{\Phi}(x, g') = -n \, g' \int \mathrm{d}^4 p \, \mathrm{d}^4 y \, f(x) \, \mathrm{e}^{-\mathrm{i}(p, x-y)} \, D_c'^{(0)}(p) \, . \quad (12.19)$$

We noted in section 6 that $f(x)$ is either a constant or a differential operator and we have therefore

$$f(x) \, \mathrm{e}^{-\mathrm{i}(p, x-y)} = f(p) \, \mathrm{e}^{-\mathrm{i}(p, x-y)} \, ,$$

where $f(p)$ is obtained from the operator $f(x)$ by the substitution

$$-\mathrm{i} \frac{\partial}{\partial x_i} \to p_i \ (i = 1, 2 \text{ or } 3) \, ; \qquad \mathrm{i} \frac{\partial}{\partial x_0} \to p_0 \, .$$

We get thus

$$\tilde{\Phi}(x, g') = -n \, g' \, (2\pi)^4 \, [f(p) \, D_c'^{(0)}(p)]_{p=0} \, , \quad (12.20)$$

and (12.18) becomes

$$\tfrac{1}{2} \, g^2 \, n^2 \, (2\pi)^4 \, V [f(p) \, D_c'^{(0)}(p)]_{p=0} \, .$$

We finally get

$$\Omega_{pf} = (2\pi)^4 \, \mathrm{i} \, V \int_0^g \frac{\mathrm{d}g'}{g'} \lim_{\substack{t\to 0 \\ t<0}} \mathrm{Tr} \int \mathrm{d}^4 p \, [M(p) \, G_c(p) \, \mathrm{e}^{-\mathrm{i}p_0 t}]'$$

$$+ \frac{g^2 \, n^2}{2} \, (2\pi)^4 \, V [f(p) \, D_c'^{(0)}(p)]_{p=0} \, . \quad (12.21)$$

We emphasise once again that one should not write down the second term on the right-hand side of (12.21) for the case of a spatially uniform system of charged particles with electromagnetic interactions. For systems of bosons interacting through a field we must change the sign of the terms containing the mass operator in (12.14) to (12.21).

b. *Direct interparticle interactions* *. The Hamiltonian of a system of particles with direct interactions is according to section 6 given by

$$H' = H'_{\mathrm{p}} + H_{\mathrm{int}} , \tag{12.22}$$

where H'_{p} and H'_{int} are given by (6.7) and (6.8), respectively.

One can also in that case obtain a formula such as (12.14) for the thermodynamic potential. We shall, however, give here an expression for Ω of a different type which enables us, in particular, to connect Ω with the eigenvalues of the effective wave equation (9.18). To do this we differentiate (12.3) with respect to β assuming all other parameters to be unchanged. We get

$$\frac{\partial \Omega}{\partial \beta} = -\beta^{-1}\,\Omega + \beta^{-1} \langle H' \rangle , \tag{12.23}$$

where, as always, $\langle H' \rangle$ is the average energy

$$\langle H' \rangle = \mathrm{Trace}\,\{ e^{\beta\Omega - \beta H'} H' \} . \tag{12.24}$$

This is clearly nothing but the internal energy of the system in the usual thermodynamic meaning of the word, and (12.23) is the usual Gibbs-Helmholtz equation.

From (12.23) we get

$$\Omega = \beta^{-1} \int_{\beta_m}^{\beta} d\beta' \, \langle H'(\beta') \rangle + C\,\beta^{-1} , \tag{12.25}$$

where the argument β' of H' under the integral sign indicates that the average must be evaluated at a temperature $T' = 1/k\beta'$, and C and β_m are constants.

We note that $\langle H' \rangle$ is a function of μ, T, and V. The thermodynamic potential Ω is the characteristic function in these variables, and we shall use $\langle H' \rangle$ and (12.25) to evaluate the thermodynamic potential.

One checks easily that as $T \to 0$ (that is, as $\beta \to \infty$) the right-hand side of (12.25) becomes the ground state energy of the system, as should be the case. Indeed, we shall evaluate the trace in the system of eigenfunctions of the Hamiltonian H' (as in sections 2 to 4 we denote the eigenvalues of H' by E_n). We get then from (12.25)

* Kogan 1959, 1960; Bonch-Bruevich 1961.

$$\Omega = \beta^{-1} \sum_n \int_{\beta_m}^{\beta} d\beta' \, e^{\beta'(\Omega - E_n)} E_n + \beta^{-1} C$$

$$= \beta^{-1} \sum_n E_n \frac{e^{\beta(\Omega - E_n)} - e^{\beta_m(\Omega - E_n)}}{\Omega - E_n} + \frac{C}{\beta} \xrightarrow[\beta \to \infty]{} E_0 .$$

We have, of course, assumed that Ω is finite, and not identically equal to zero.

The problem of evaluating Ω is through (12.25) reduced to that of finding the average energy $\langle H' \rangle$. From (6.7) and (6.8) we get

$$\langle H' \rangle = \int d\lambda \, d\lambda' (\lambda' | T+V-\mu | \lambda) \langle a^+(\lambda') a(\lambda) \rangle$$

$$+ \tfrac{1}{2} \int d\lambda' \, d\lambda_1 \, d\lambda_2 \, d\lambda_3 (\lambda', \lambda_1 | U | \lambda_3, \lambda_2) \langle a^+(\lambda') a^+(\lambda_1) a(\lambda_2) a(\lambda_3) \rangle . \quad (12.26)$$

Using (5.2) and (7.6) we can rewrite this as follows

$$\langle H' \rangle = i \int d\lambda \, d\lambda' (\lambda' | T+V-\mu | \lambda) \lim_{\substack{x_0' \to x_0 \\ x_0' > x_0}} G_c(\lambda, x_0; \lambda', x_0')$$

$$+ \frac{i}{2} \int d\lambda' \, d\lambda_1 \, d\lambda_2 \, d\lambda_3 (\lambda', \lambda_1 | U | \lambda_3, \lambda_2) \lim_{\substack{x_0' \to x_0 \\ x_0' > x_0}} G_{2,c}(\lambda_1, \lambda_2, \lambda_3, x_0; \lambda', x_0') . \quad (12.27)$$

We use (7.7) to express the Green function $G_{2,c}$ in terms of the single-particle Green function and its time derivative. When $x_0' \neq x_0$ we have

$$\int d\lambda' \, d\lambda_1 \, d\lambda_2 \, d\lambda_3 (\lambda', \lambda_1 | U | \lambda_3, \lambda_2) \, G_{2,c}(\lambda_1, \lambda_2, \lambda_3, x_0; \lambda', x_0')$$

$$= \int d\lambda' \left\{ i \frac{\partial G_c(\lambda', x_0; \lambda', x_0')}{\partial x_0} - \int d\lambda (\lambda' | T+V-\mu | \lambda) \, G_c(\lambda, x_0; \lambda', x_0') \right\} .$$

We substitute this expression into (12.27) and write G_c as a Fourier integral over the time. We then get

$$\langle H' \rangle = \frac{i}{2} \lim_{\substack{t \to 0 \\ t < 0}} \int_{-\infty}^{+\infty} dE \, e^{-iEt} \int d\lambda' \, \{ E \, G_c(\lambda', \lambda'; E)$$

$$+ \int d\lambda (\lambda' | T+V-\mu | \lambda) \, G_c(\lambda, \lambda'; E) \} . \quad (12.28)$$

This formula becomes especially simple when the operator $T+V-\mu$ is diagonal. Let its eigenvalues be $W(\lambda) - \mu$. The second term on the right-hand side of (12.28) is then

$$\frac{i}{2}\lim_{\substack{t\to 0\\ t<0}}\int_{-\infty}^{+\infty} dE\ e^{-iEt}\int d\lambda\,[W(\lambda)-\mu]\,G_c(\lambda,\lambda;E)=\tfrac{1}{2}\int d\lambda\,n(\lambda)\,[W(\lambda)-\mu].$$

We have used here (5.4) to write

$$n(\lambda)=i\lim_{\substack{t\to 0\\ t<0}}\int_{-\infty}^{+\infty} dE\ e^{-iEt}\,G_c(\lambda,\lambda;E)$$

for the distribution function in λ, normalised to the occupation number.

We get thus

$$\langle H'\rangle=\tfrac{1}{2}\int d\lambda\,n(\lambda)\,W(\lambda)-\frac{\mu N}{2}+\frac{i}{2}\lim_{\substack{t\to 0\\ t<0}}\int_{-\infty}^{+\infty} dE\ e^{-iEt}\int d\lambda\,E\,G_c(\lambda,\lambda;E)\ , \tag{12.29}$$

where N is the total number of particles in the system.

One can easily convince oneself that this formula is also valid for boson systems; the calculation is completely similar to the one for the fermion case.

In the spatially uniform case when we can put $V(\vec{x})=0$, the variable λ indicates the spin quantum number s and the three components of the momentum $\vec{p}$. We get then from (12.29) *

$$\frac{\langle H'\rangle}{V}=-\frac{n\mu}{2}+\frac{i}{2}\,\mathrm{Tr}\int d^3\vec{p}\lim_{\substack{t\to 0\\ t<0}}\int_{-\infty}^{+\infty} dE\ e^{-iEt}[W(\vec{p})+E]\,G_c(\vec{p},E)\ . \tag{12.30}$$

Here V is the volume of the system (not to be confused with the potential energy of the particles in an external field $V(\vec{x})$!) and the sumbol Tr indicates as always the trace over the spin coordinates. As $T\to 0$, (12.30) becomes the expression for the ground state energy obtained by a number of authors (Galitskiĭ and Migdal 1958, Belyaev 1958a, Hugenholtz and Pines 1959; we have used Hugenholtz and Pines' method here).

If the bilinear expansions (9.26) and (9.32) are valid, (12.29) enables us to express the average energy (and thus the thermodynamic potential) in terms of the eigenvalues of the effective wave equation (9.18). Indeed, substituting (9.26) or (9.32) into (12.29) we get easily

* We must bear in mind that $G_c(\vec{p},\vec{p}';E)=\delta(\vec{p}-\vec{p}')\,G_c(\vec{p},E)$; when the arguments of the δ-function are the same we must interpret that in this case as the volume of the system divided by $(2\pi)^3$. One can also obtain (12.30) easily by writing (12.27) in the coordinate representation and then expanding $G_c(\vec{x},\vec{x}';E)$ in a Fourier integral with respect to the position coordinates.

$$\langle H' \rangle = \tfrac{1}{2} \int d\lambda\, n(\lambda) \left[W(\lambda) - \mu \right] + \tfrac{1}{2} \int dE\, dv\, \frac{Z(E, v) E}{e^{\beta E} \pm 1}$$

$$= \int dE\, dv\, \frac{E Z(E, v)}{e^{\beta E} \pm 1} - \tfrac{1}{2} \int d\lambda\, dE\, dv\, \frac{Z(E, v)}{e^{\beta E} \pm 1}$$

$$\times \chi^{+}(\lambda, E, v) \left[R - W(\lambda) - \mu \right] \chi(\lambda, E, v) \,. \qquad (12.31)$$

In the denominators the plus-(minus-)sign refers to the fermion (boson) case. We have used here

$$n(\lambda) = \int dE\, dv\, \frac{Z(E, v)}{e^{\beta E} \pm 1} \left| \chi(\lambda, E, v) \right|^2 \,. \qquad (12.32)$$

The integration over E in (12.31) is over the whole spectrum of the effective wave equation (9.18). We note that because of (9.29) the integrals over E and v in (12.31) are proportional to the total number of particles in the system, as should, of course, be the case.

We can get yet another useful way of writing the average energy, by regrouping slightly the terms in (12.26), and writing

$$\langle H' \rangle = \int d\lambda\, d\lambda' (\lambda' \left| T + V - \mu \right| \lambda) \langle a^{+}(\lambda') a(\lambda) \rangle$$

$$+ \int d\lambda'\, d\lambda_1\, d\lambda_2\, d\lambda_3\ (\lambda', \lambda_1 | U | \lambda_3, \lambda_2) \langle a^{+}(\lambda') a^{+}(\lambda_1) a(\lambda_2) a(\lambda_3) \rangle$$

$$- \tfrac{1}{2} \int d\lambda'\, d\lambda_1\, d\lambda_2\, d\lambda_3 (\lambda', \lambda_1 | U | \lambda_3, \lambda_2) \langle a^{+}(\lambda') a^{+}(\lambda_1) a(\lambda_2) a(\lambda_3) \rangle \,.$$

We transform the first two terms as before and get (compare (12.28))

$$i \lim_{\substack{t \to 0 \\ t < 0}} \int_{-\infty}^{+\infty} dE\, e^{-iEt} \int d\lambda\, E\, G_c(\lambda, \lambda; E) \,, \qquad (12.33)$$

where λ is an arbitrary variable. When (9.16) can be applied, this expression can be written as follows (compare (12.31))

$$\int dE\, dv\, \frac{E Z(E, v)}{e^{\beta E} \pm 1} = V \int dE\, dv\, \frac{Z'(E, v) E}{e^{\beta E} \pm 1} \,, \qquad (12.34)$$

where the plus-(minus-)sign refers again to the fermion (boson) case. Here Z' is defined by (9.29) and the integral on the right-hand side of (12.34) is independent of the volume of the system V, asymptotically as $V \to \infty$. To transform the last term - which we shall denote by A for the time being - it is convenient to use the coordinate representation. We have then

$$A = -\tfrac{1}{2}\int \mathrm{d}^3\vec{x}\,\mathrm{d}^3\vec{x}'\; U(\vec{x}-\vec{x}')\,\langle a^+(\vec{x})a^+(\vec{x}')a(\vec{x}')a(\vec{x})\rangle$$

$$= \tfrac{1}{2}\int \mathrm{d}^3\vec{x}\,\mathrm{d}^3\vec{x}'\; U(\vec{x}-\vec{x}')\,\langle -a^+(\vec{x}')a(\vec{x}')a^+(\vec{x})a(\vec{x}) + \delta(\vec{x}-\vec{x}')a^+(\vec{x})a(\vec{x})\rangle$$

$$= \tfrac{1}{2}\,U(0)\,N - \frac{\mathrm{i}}{2}\lim_{\substack{x_0'\to x_0\\ x_0'>x_0}}\int \mathrm{d}^3\vec{x}\,\mathrm{d}^3\vec{x}'\; U(\vec{x}-\vec{x}')\,G_{2,c}(x,x')\ .$$

Here $G_{2,c}(x,x')$ is defined by (5.24) with $x_1 = x_2 = x$, $x_1' = x_2' = x'$ (it should not be confused with $G_{2,c}(\lambda_1,\lambda_2,\lambda_3,x_0;\lambda',x_0')$ defined by (7.6): the arguments are distributed differently in that case). In a system of charged particles $U(\vec{x})$ tends to infinity as $\vec{x}\to 0$; the corresponding contribution is, however, not an interaction energy term, but a self-energy term and we must drop it. This can be done formally by introducing instead of $U(\vec{x})$ a regularised expression in the same way as is done in quantum electrodynamics by the limiting λ-process (Wentzel 1947) *. If we drop the term $\frac{1}{2}N\,U(0)$ and introduce in the usual manner the Fourier transform $G_{2,c}(\vec{x},\vec{x}';E)$, we get

$$A = -\frac{\mathrm{i}}{2}\lim_{\substack{t\to 0\\ t<0}}\int_{-\infty}^{+\infty}\mathrm{d}E\;\mathrm{e}^{-\mathrm{i}Et}\int \mathrm{d}^3\vec{x}\,\mathrm{d}^3\vec{x}'\; U(\vec{x}-\vec{x}')\,G_{2,c}(\vec{x},\vec{x}';E)\ . \quad (12.35)$$

One can easily integrate over E, if the bilinear expansion (9.44) is applicable, and one gets from (12.35)

$$A = \tfrac{1}{2}\int \mathrm{d}E\,\mathrm{d}v\; Z_2(E,v)\,n_B(E)$$
$$\int \mathrm{d}^3\vec{x}\,\mathrm{d}^3\vec{x}'\; U(\vec{x}-\vec{x}')\,\chi_2(\vec{x},\vec{x};E,v)\,\chi_2^+(\vec{x}',\vec{x}';E,v)\ . \quad (12.36)$$

We now write

$$\tfrac{1}{2}\,Z_2(E,v)\int \mathrm{d}^3\vec{x}\,\mathrm{d}^3\vec{x}'\; U(\vec{x}-\vec{x}')\,\chi_2(\vec{x},\vec{x};E,v)\,\chi_2^+(\vec{x}',\vec{x}';E,v)$$
$$= V\,E\,Z_2'(E,v)\ . \quad (12.37)$$

Combining (12.34), (12.36), and (12.37) we find finally

* Take, for instance,

$$U(\vec{x}) = \frac{e^2}{r} = \frac{e^2}{2\pi^2}\int \mathrm{d}^3\vec{k}\;\frac{\mathrm{e}^{\mathrm{i}(\vec{k}.\vec{x})}}{\vec{k}^2}\quad (r = |\vec{x}|)\ .$$

We replace the Fourier coefficient $1/(2\pi^2\vec{k}^2)$ by the regularised expression $\cos k\lambda/(2\pi^2\vec{k}^2)$, where λ is a small, positive constant. We then get

$$U_{\mathrm{reg}} = \frac{e^2}{2r}\left(1 + \frac{r-\lambda}{|r-\lambda|}\right)\xrightarrow[\lambda\to 0]{}\begin{cases}\dfrac{e^2}{r}\ , & r\neq 0\ ,\\ 0\ , & r = 0\ .\end{cases}$$

$$\frac{\langle H' \rangle}{V} = \int \mathrm{d}E\ \mathrm{d}v\ \frac{EZ'(E, v)}{\mathrm{e}^{\beta E} \pm 1} + \mathrm{d}E'\ \mathrm{d}v'\ \frac{E'Z_2'(E', v')}{\mathrm{e}^{\beta E'} - 1} . \qquad (12.38)$$

The first term is formally the same as the expression for the average energy per particle of a perfect (fermion or boson) gas; the second term is formally the average energy per particle of some perfect boson gas. We remind ourselves in this connexion that the variables v, E and v', E' in the first and the second term have in general different meanings (see (9.26) and (9.44)). The domains of integration over E and E' are also different. Since the spectral function corresponding to $G_{2,c}$ is volume-independent, asymptotically as $V \to \infty$, the same is true for Z_2'.

From (12.25) (with $\beta_m \to 0$) and (12.38) we get for the thermodynamic potential

$$\frac{\Omega}{V} = C\ \beta^{-1} - \beta^{-1} \int_{\beta}^{\infty} \mathrm{d}\beta' \left\{ \int \mathrm{d}E\ \mathrm{d}v\ \frac{EZ'(E, v)}{\mathrm{e}^{\beta' E} \pm 1} + \int \mathrm{d}E'\ \mathrm{d}v'\ \frac{E'Z_2'(E', v')}{\mathrm{e}^{\beta' E'} - 1} \right\} . \qquad (12.39)$$

It has been shewn (Luttinger and Ward 1960, Klein 1961 *) that under certain conditions $\delta\Omega/\delta M = 0$. In that case (12.39) becomes the usual formula for the thermodynamic potential of two perfect gases:

$$\frac{\Omega}{V} = \frac{C'}{\beta} + \beta^{-1} \int \mathrm{d}E\ \mathrm{d}v\ Z'(E, v) \ln (1 \pm \mathrm{e}^{-\beta E}) + \int \mathrm{d}E'\ \mathrm{d}v'\ Z_2'(E', v') \ln (1 - \mathrm{e}^{-\beta E'}) , \qquad (12.40)$$

where the upper (lower) sign refers to the fermion (boson) case.

One can also obtain expressions such as (12.25) and (12.31) for the thermodynamic potential of a system of particles interacting through a quantum field. We find in that case, proceeding exactly as before, and assuming (9.26) to be applicable,

$$\langle H' \rangle = \langle H_p' \rangle + \langle H_f \rangle + \langle H_{pf} \rangle = \int \mathrm{d}E\ \mathrm{d}v\ \frac{EZ(E, v)}{\mathrm{e}^{\beta E} \pm 1} + \langle H_f \rangle , \qquad (12.41)$$

where E denotes the eigenvalues of the effective wave equation for the corpuscular Green function. The average $\langle H_f \rangle$ can also be expressed in terms of Green functions; it is, however, for systems of this kind apparently more convenient to use (12.21).

In conclusion we note that in the method developed here there are no difficulties about the volume-dependence of Ω (or of the ground

* The authors express their thanks to A. Klein for sending them a preprint of this paper.

state energy E_0). Indeed, we noted in section 10 that the equations for the Green functions are volume-independent as $V \to \infty$. The complete volume-dependence is thus asymptotically given by the factor V in such formulae as (12.21) and (12.30). We can thus immediately determine the specific quantities which are asymptotically volume-independent, such as the thermodynamic potential per unit volume or per particle, and we have thus solved the second problem formulated in the Introduction.

13. CORRELATION FUNCTIONS *

We can use the results of sections 1 to 3 to express different kinds of correlation functions directly in terms of limiting values of the appropriate Green functions. In the present section we shall consider some expressions for the correlation functions in terms of functional derivatives; we shall also study in some detail the current time correlation function which is important for the following discussions.

From (5.2) and (1.2) we have

$$G_c(\lambda, x_0; \lambda', x_0') = \mathrm{i}\,\mathrm{Trace}\, e^{\beta\Omega - \beta H'}\, T\{a(\lambda, x_0) a^+(\lambda', x_0')\} . \quad (13.1)$$

We remind ourselves of the fact that H' is a generalised Hamiltonian

$$H' = H - \mu N .$$

We write the total particle number operator N occurring here as follows:

$$N = \int d\lambda''\, a^+(\lambda'', x_0) a(\lambda'', x_0') . \quad (13.2)$$

The two operators H and N must be taken at the same time, but it is immaterial at what time: we consider as always the case where H and N, taken at the same time, commute. We shall make in (13.1) the formal substitution $\beta\mu \to F(\lambda'', \lambda''') + \beta\mu$, or, accordingly,

$$\beta\mu N \to \beta\mu N + \int d\lambda''\, d\lambda'''\, F(\lambda'', \lambda''')\, a^+(\lambda'', x_0)\, a(\lambda''', x_0) . \quad (13.3)$$

The function obtained in this way we denote by $G_c'(F)$; we have clearly

$$G_c(\lambda, x_0; \lambda', x_0') = \lim_{F \to 0} G_c'(\lambda, x_0; \lambda', x_0'; F) . \quad (13.4)$$

To simplify our formulae we shall in the remainder of this section simply write lim, without explicitly indicating the condition $F \to 0$.

* Bonch-Bruevich 1959a, b, Hugenholtz and Pines 1959.

It is immediately clear that the functional derivative of G' with respect to F gives, first of all, a term of the form $\beta G'\,\delta\Omega/\delta F(\lambda'', \lambda''')$ and, secondly, a higher order Green function with four operators a^+, a under the averaging sign *. The latter is connected with the operator ρ_2; we find thus easily, after taking the limit $(F \to 0)$:

$$(\lambda_1, \lambda_2 \mid \rho_2 \mid \lambda_2', \lambda_1') = \Big[\rho_1(\lambda_1', \lambda_2')\ \rho_1(\lambda_2, \lambda_1) - \delta(\lambda_1' - \lambda_2)\ \rho_1(\lambda_1', \lambda_1) + \lim \frac{\delta \rho_1'(\lambda_2, \lambda_1)}{\delta F(\lambda_1', \lambda_2')}\Big]_{a,s} . \tag{13.5}$$

The symbol $[\ldots]_{a,s}$ indicates here that the expression within the brackets must be antisymmetrised or symmetrised with respect to the variables λ_1', λ_2' and λ_1, λ_2 depending on whether the operators a^+, a are fermion or boson operators; the function ρ_1' is connected with G_c' in the same way as ρ_1 with G_c. The matrix ρ_2 describes the correlation with respect to the arbitrary variable λ at a given time.

We shall, in particular, consider the momentum correlation function in a spatially uniform and isotropic system without spin interactions. It is convenient then to choose for λ the three momentum components $\vec{p}$ and the spin coordinate s. We use a discrete momentum representation (that is, we shall assume that the system is enclosed within a large "periodicity cube" of volume V) and we introduce the average occupation number $n(\vec{p}, s)$ of the state $(\vec{p}, s)$. The matrix ρ_1 is here clearly diagonal in the spin variable and we use instead of (13.3) the substitution

$$\beta\mu N \to \beta\mu N + \sum_{\vec{p},s} F(\vec{p}, s)\ a^+(\vec{p}, s)\ a(\vec{p}, s) .$$

We get then from (13.5)

$$\rho_2(\vec{p}', s'; \vec{p}, s) \equiv \langle a^+(\vec{p}', s')\ a^+(\vec{p}, s)\ a(\vec{p}, s)\ a(\vec{p}', s')\rangle$$

$$= n(\vec{p}, s)\ a(\vec{p}', s') - \Delta(\vec{p}' - \vec{p})\ \Delta(s' - s)\ n(\vec{p}, s) + \lim \frac{\partial n'(\vec{p}, s)}{\partial F(\vec{p}', s)} , \tag{13.6}$$

where Δ is a delta-function of a discrete argument. For a perfect electron gas, when the occupation number is the usual Fermi function, (13.6) becomes, in particular,

$$\rho_2(\vec{p}', s'; \vec{p}, s) = n(\vec{p}, s)\ n(\vec{p}', s') - \Delta(\vec{p} - \vec{p}')\ \Delta(s - s')\ n^2(\vec{p}, s) . \tag{13.7}$$

The second term on the right-hand side of (13.7) describes the "kinematic" correlation connected with the Pauli principle: the probability to observe two electrons with the same momentum and spin is zero. Otherwise the electrons move, of course, independently of one an-

* This is a particular case of the general two-particle Green function, corresponding to a special arrangement of the operators a^+, a over the time coordinates.

other (perfect gas). When there are interactions, the distribution function $n(\vec{p},s)$ will in general be more complicated; one can see from (13.6) that there is then an additional (dynamical) momentum correlation which is caused by the interactions.

Similarly we can use the substitution

$$\beta\mu N \to \beta\mu N + \int F(\lambda'',\lambda''';x_0'',x_0''')\, a^+(\lambda'',x_0'')\, a(\lambda''',x_0''')\, d\lambda''\, d\lambda'''\, dx_0''\, dx_0'''$$

to obtain an expression for the time-correlation functions. One can also immediately generalise this to the case of many-particle correlation functions (one must clearly in that case take higher order functional derivatives of G').

We can obtain yet another useful way of writing the pair-correlation function in terms of the functional derivative of the thermodynamic potential Ω with respect to the interaction potential for the case of systems with direct interactions. Indeed, we have in that case from (12.3), (12.22), (6.7), and (6.8)

$$\Omega = -\beta^{-1} \ln \mathrm{Trace} \exp\{-\beta H_p' - \frac{\beta}{2}\int d\lambda_1\, d\lambda_2\, d\lambda_1'\, d\lambda_2' (\lambda_1,\lambda_2|U|\lambda_2',\lambda_1')\, a^+(\lambda_1)\, a^+(\lambda_2)\, a(\lambda_2')\, a(\lambda_1')\} \tag{13.8}$$

(all operators a^+,a refer to the same time, and it is immaterial what that time is). From this we get

$$\frac{\delta\Omega}{\delta(\lambda_1,\lambda_2|U|\lambda_2',\lambda_1')} = \tfrac{1}{2}\langle a^+(\lambda_1)\, a^+(\lambda_2)\, a(\lambda_2')\, a(\lambda_1')\rangle \equiv \tfrac{1}{2}\rho_2(\lambda_1',\lambda_2';\lambda_2,\lambda_1) . \tag{13.9}$$

This equation is particularly convenient to evaluate coordinate correlation functions in a spatially uniform system. In that case it is convenient to choose for λ the spin and the three spatial coordinates; the interaction energy operator is now

$$H_{\mathrm{int}} = \tfrac{1}{2}\int d^3\vec{x}\, d^3\vec{x}' \sum_{s,s'} a^+(\vec{x},s)\, a^+(\vec{x}',s')\, U(\vec{x},\vec{x}')\, a(\vec{x}',s')\, a(\vec{x},s) , \tag{13.10}$$

and we have thus

$$\frac{\delta\Omega}{\delta U(\vec{x},\vec{x}')} = \tfrac{1}{2}\sum_{s,s'}\langle a^+(\vec{x},s)\, a^+(\vec{x}',s')\, a(\vec{x}',s')\, a(\vec{x},s)\rangle \equiv \tfrac{1}{2}\frac{N^2}{V} f(\vec{x}-\vec{x}') , \tag{13.11}$$

where

$$f(\vec{x}-\vec{x}') = \frac{V}{N^2}\sum_{s,s'}\langle a^+(\vec{x},s)\, a^+(\vec{x}',s')\, a(\vec{x}',s')\, a(\vec{x},s)\rangle . \tag{13.12}$$

The function $f(\vec{x}-\vec{x}')$ describes the correlation in coordinate space; the constant factor on the right-hand side of (13.12) is chosen such that the integral $\int f(\vec{x})\, d^3\vec{x}$ be a finite quantity which is independent of N and V asymptotically (as $N \to \infty$, $V \to \infty$, $0 < N/V = n < \infty$). We have thus

$$f(\vec{x}) = \frac{2V}{N^2} \frac{\delta\Omega}{\delta U(\vec{x})} . \tag{13.13}$$

We can use one of the equations from the preceding section for the thermodynamic potential Ω.

We note, in particular, the case where the direct pair-interaction is replaced by an interaction through an effective quantum field, the Green function of which is defined by (I.62). The thermodynamic potential Ω is then given by (12.4) and (12.21). We put

$$D_c^{(0)}(\vec{k}) = \frac{1}{(2\pi)^3} \int D_c^{(0)}(\vec{x})\, e^{-i(k,x)}\, d^3\vec{x} .$$

Using (12.15a) and performing the variation implied in (13.13) we get

$$f(\vec{x}) = i \frac{V^2}{N^2 g^2} \int_0^g \frac{dg'}{g'} \int d^3\vec{k}\, e^{i(\vec{k}.\vec{x})}$$

$$\times \frac{\delta}{\delta D_c^{(0)}(k)} \lim_{\substack{t\to 0 \\ t<0}} \int d^4k'\, e^{-ik'_0 t} \left[\mathcal{P}(k',g')\, D_c(k',g')\right]' + \frac{V^2}{N^2} . \tag{13.14}$$

One should not write down the last term in the case of systems of charged particles with electromagnetic interactions.

It is clear from (13.14) that the Fourier transform of the correlation function $f(\vec{x})$ ultimately is determined by the poles of the Green function D_c. We know, however, that these poles determine some of the branches of the elementary excitation spectrum in the system. There is thus an important connexion between the form of the correlation function and the excitation spectrum *.

Up to this point we have in this section considered only "single-time" correlation functions which characterise the connexion between the probabilities of observing various quantities taken all at the same time. We shall now consider one particular case of double-time correlation functions, namely the correlation function for two components of the current density ** taken at different times:

$$F_{il}^{(+)}(x, x') = \langle [j_i(x), j_l(x')]_+ \rangle . \tag{13.15}$$

* Feynman (1954) was the first to note this connexion for the case of liquid helium II.

** We consider here only the conductivity current, and not the spin current.

We shall need this quantity later on in the theory of electrical conductivity. We restrict ourselves to the spatially uniform and isotropic case. When we apply our formula to solids, this latter restriction means a restriction to cubic crystals. We have then

$$F_{il}^{(+)}(x, x') = \int_{-\infty}^{+\infty} dE \int d^3\vec{k}\; e^{-iE(x_0 - x_0') + i(\vec{k}.\vec{x} - \vec{x}')}\, F_{il}^{(+)}(\vec{k}, E) \; . \quad (13.16)$$

As the operator $j_i(x)$ is Hermitean, we have clearly

$$F_{il}^{(+)}(\vec{k}, E) = F_{li}^{(+)}(-\vec{k}, -E) = F_{li}^{(+)+}(\vec{k}, E) \; . \quad (13.17)$$

Because of (4.2) we have, moreover,

$$F_{il}^{(+)}(\vec{k}, E) \in \mathrm{Re} \; ; \quad F_{il}^{(+)}(\vec{k}, E) > 0 \; ; \quad F_{il}^{(+)}(\vec{k}, E) = F_{li}^{(+)}(\vec{k}, E) \; . \quad (13.18)$$

We can thus write $F_{il}^{(+)}(\vec{k}, E)$ in the form

$$F_{il}^{(+)}(\vec{k}, E) = \delta_{il}\, F_1(\vec{k}^2, E^2) + (k_i\, k_l - \vec{k}^2\, \delta_{il})\, F_2(\vec{k}^2, E) \; , \quad (13.19)$$

where

$$F_1 - k^2\, F_2 \geq 0 \; , \qquad F_2 \geq 0 \quad (13.20)$$

(and thus $F_1 \geq 0$). Because of the charge conservation law $F_1(\vec{k}^2, E^2)$ satisfies an important identity (Kubo 1957, Martin and Schwinger 1959). We get this equation using the connexion between $F_{il}^{(+)}(\vec{k}, E)$ and the current density commutator, the equation of continuity, and the well-known commutation relations for the charge density and the current density, taken at the same moment. First of all we get by using (2.10)

$$\begin{aligned} \langle [j_i(x), j_l(x')]_- \rangle &= \int_{-\infty}^{+\infty} dE \int d^3\vec{k}\; e^{-iE(x_0 - x_0') + i(\vec{k}.\vec{x} - \vec{x}')} \tanh \frac{\beta E}{2}\, F_{il}^{(+)}(\vec{k}, E) \\ &= i \frac{\partial}{\partial x_0} \int_{-\infty}^{+\infty} dE \int d^3\vec{k}\; e^{-iE(x_0 - x_0') + i(\vec{k}.\vec{x} - \vec{x}')} \frac{\tanh \frac{\beta E}{2}}{E}\, F_{il}^{(+)}(\vec{k}, E) \; . \end{aligned} \quad (13.21)$$

We shall, moreover, denote by $\rho(x)$ the charge density operator *. From the equation of continuity we get

$$\frac{\partial}{\partial x_i} \langle [j_i(x), j_l(x')]_- \rangle = - \langle [\frac{\partial \rho(x)}{\partial x_0}, j_l(x')]_- \rangle \; . \quad (13.22)$$

Combining this with (13.21) and (13.19), we get

* There should be no confusion with the operators $\rho_1, \rho_2, \ldots,$ as these have always indices $1, 2, \ldots, s$.

$$<[\rho(x), j_l(x')]_->$$
$$= -i\frac{\partial}{\partial x_l}\int_{-\infty}^{+\infty} dE \int d^3\vec{k}\, e^{-iE(x_0-x_0')+i(\vec{k}.\vec{x}-\vec{x}')}\frac{\tanh\frac{\beta E}{2}}{E}F_1(\vec{k}^2,E^2)\,. \tag{13.23}$$

We now put in (13.23) $x_0' = x_0$. The commutator on the left-hand side can then easily be evaluated.

We consider, first of all, the simplest case when the velocity operator is simply $\vec{p}/m_0$, where m_0 is the true particle mass. We have then

$$<[\rho(\vec{x}, x_0), j_l(\vec{x}', x_0)]_-> = -\frac{ine^2}{m_0}\frac{\partial\delta(\vec{x}-\vec{x}')}{\partial x_l}\,, \tag{13.24}$$

where $n = <\rho(\vec{x})>$ is the particle density which is constant as we are considering a uniform system.

The result (13.24) is, however, valid only when there are no external fields. It is impossible to use it in solid state theory where the quantity n is not a constant but a periodic function of the coordinates, because of the periodic field of the lattice. It is possible for a number of solid state problems to eliminate the periodic lattice potential explicitly from our considerations (Pekar 1946b, Slater 1949, Kittel and Mitchell 1954, Luttinger and Kohn 1955) by replacing the usual kinetic energy operator $\vec{p}^2/2m_0$ by an operator $T(\vec{p})$ which is the energy of an electron in the periodic lattice field. In this case $\vec{p}$ is the quasi-momentum of the electron; when we change to the coordinate representation $\vec{p}$ must be replaced by $-i\nabla_{\vec{x}}$. If there are no lattice defects, the system becomes then (formally) spatially uniform, and n is a constant, but in return the velocity is given by the formula

$$v_i(\vec{p}) = \frac{\partial T(\vec{p})}{\partial p_i}\left(\neq\frac{p_i}{m_0}\right).$$

The velocity $\vec{v}$ is, in general, not parallel to the vector $\vec{p}$, even not in a cubic crystal, as the surface $T(\vec{p})$ = constant may have preferred directions. From symmetry considerations it is clear that only the average of $v_l(\vec{p})$ over such directions may occur in the expression for the current density j_l. It is clear that it can be written in the form $p_l f(\vec{p}^2)$, where $f(\vec{p}^2)$ is a scalar function (in the particular case when $T(\vec{p}) = \vec{p}^2/2m_0$, we have $f = 1/m_0$). We get then for the commutator in which we are interested

$$<[\rho(\vec{x}, x_0), j_l(\vec{x}', x_0)]_-> = -ine^2 f(-\nabla^2_{\vec{x}})\frac{\partial\delta(\vec{x}-\vec{x}')}{\partial x_l}\,, \tag{13.24a}$$

and thus

$$ne^2 f(-\nabla^2_{\vec{x}})\,\delta(\vec{x}-\vec{x}') = \int_{-\infty}^{+\infty} dE \int d^3\vec{k}\, e^{i(\vec{k}.\vec{x}-\vec{x}')}\frac{\tanh\frac{\beta E}{2}}{E}F_1(\vec{k}^2,E^2)\,.$$

Since $f(-\nabla^2_{\vec{x}})\, e^{i(\vec{k}.\vec{x})} = f(\vec{k}^2)\, e^{i(\vec{k}.\vec{x})}$ we get

$$\int_{-\infty}^{+\infty} dE \frac{\tanh \frac{\beta E}{2}}{E} F_1(\vec{k}^2, E^2) = \frac{ne^2}{(2\pi)^3} f(\vec{k}^2) . \qquad (13.25)$$

Let us, in particular, consider the case where the energy depends quadratically on the quasi-momentum,

$$T(\vec{p}) = \sum_{i=1}^{3} \frac{(p_i - p_i^{(0)})^2}{2m_i} . \qquad (13.26)$$

In (13.26) the $p_i^{(0)}$ are given numbers which determine the position of the energy minima in the Brillouin zone, and the m_i are the principal values of the effective mass tensor. If we use this expression to evaluate the components of the velocity $v_l(\vec{p})$, and perform the average mentioned above, we find

$$f(\vec{p}^2) = \frac{1}{m^*} \equiv \frac{1}{3} \sum_{i=1}^{3} \frac{1}{m_i} . \qquad (13.27)$$

We get then from (13.25)

$$\int_{-\infty}^{+\infty} dE \frac{\tanh \frac{\beta E}{2}}{E} F_1(\vec{k}^2, E^2) = \frac{1}{(2\pi)^3} \cdot \frac{ne^2}{m^*} . \qquad (13.28)$$

One should note that the right-hand side of (13.28) is independent of $\vec{k}$. Equation (13.25) is the relation we were looking for. We derived it, assuming that there was only one kind of charged particles; a generalisation to the case of several kinds is obtained by replacing the right-hand side of (13.25) by

$$\frac{1}{(2\pi)^3} \sum_a n_a e_a^2 f_a(\vec{k}^2) .$$

The index a enumerates here the different kinds of particles and the summation is over all values it can take on. In the next section we shall use (13.25) as a starting point for a "sum rule" in the theory of electrical conductivity.

We note in conclusion that once we know $F_{il}^{(+)}(x,x')$ we can also determine the time-correlation function for the charge densities. Indeed, from the equation of continuity we have (compare (13.22))

$$\frac{\partial^2}{\partial x_l' \partial x_i} \langle [j_i(x), j_l(x')]_+ \rangle = \langle [\frac{\partial \rho(x)}{\partial x_0} , \frac{\partial \rho(x')}{\partial x_0}]_+ \rangle ,$$

and hence

$$\langle [\rho(x), \rho(x')]_+ \rangle = \int_{-\infty}^{+\infty} dE \int d^3\vec{k}\, e^{-iE(x_0 - x_0') + i(\vec{k}.\vec{x} - \vec{x}')} \frac{\vec{k}^2}{E^2} F_1(\vec{k}^2, E^2) . \qquad (13.29)$$

14. THE REACTION OF A SYSTEM TO EXTERNAL ACTION; REPRESENTATION THROUGH DOUBLE-TIME GREEN FUNCTIONS *

In the present and the next section we shall shew that once we know the simplest Green function, defined under conditions of thermodynamic equilibrium, we are able to study not only the equilibrium properties of the system, but also the quantities which characterise its reaction to any kind of external action. In particular, it turns out to be possible to evaluate the charge, energy, ... current densities which occur in the system when there are electrical fields, ... applied. In this way we obtain closed expressions for the electrical conductivity and other transport coefficients.

We shall restrict ourselves to the case of small deviations from equilibrium, consider the external action as a perturbation, and evaluate the averages of all quantities of interest to us only in the first non-vanishing approximation.

Let the system initially be in thermodynamic equilibrium and let there be adiabatically switched on an external perturbation acting upon it. It is convenient to take the initial time to be $-\infty$; we can then write that part of the Hamiltonian, ΔH, which describes the interaction between the system and the perturbation as

$$\Delta H = - A_m \, e^{-i\omega x_0 - \varepsilon |x_0|} \, C_1 , \tag{14.1}$$

where A_m is a c-number (the "amplitude" of the external field) and C_1 is an operator depending on the nature of the interaction, but independent of λ. Usually, C_1 contains an integral over λ (vide infra). Choosing ΔH to be a harmonically oscillating function as given by (14.1) does not violate the general nature of our considerations as long as we restrict ourselves to the first approximation which is linear in ΔH.

One can easily find the average of an operator $C_2(x)$ when there is a perturbation by using the general formula (1.2) if we take the perturbation (14.1) into account when evaluating the density matrix ρ. We denote by H' the Hamiltonian of the system when there is no perturbation. From (1.3) we get

$$i \frac{\partial \rho}{\partial x_0} = H' \rho - \rho H' + \Delta H \rho - \rho \Delta H . \tag{14.2}$$

Let ρ_0 be the density matrix characterising the system in thermodynamic equilibrium when there is no perturbation. We shall for the sake of simplicity call it in the following simply the equilibrium density matrix. We have clearly $[\rho_0, H']_- = 0$. We put

$$\rho = \rho_0 + \Delta\rho , \tag{14.3}$$

* Kubo 1957, Martin and Schwinger 1959, Klinger 1959, Zubarev 1960, Tyablikov 1960.

and restrict ourselves to terms of first order in $\Delta\rho$ and ΔH. Using the boundary condition $\rho \xrightarrow[x_0 \to -\infty]{} \rho_0$ we get from (14.2)

$$\Delta\rho = -i\int_{-\infty}^{x_0} e^{-iH'(x_0-x_0')}\,[\Delta H,\ \rho_0]_-\,e^{iH'(x_0-x_0')}\,dx_0' . \quad (14.4)$$

We find thus for the average of the operator $C_2(x_0)$ at time x_0 from (1.2)

$$\tilde{C}(x_0) = \tilde{C}_2^{(0)}(x_0) - i\int_{-\infty}^{x_0} \langle [C_2(x_0),\ \Delta H(x')]_- \rangle\, dx_0' . \quad (14.5)$$

Here $\tilde{C}_2^{(0)}$ is the average of C_2 when there is no perturbation (when $A_m = 0$) and we consider operators which are Heisenberg operators with respect to the unperturbed Hamiltonian H'. To simplify our formulae we have not explicitly indicated the parameters λ on which C_2 may depend, but only its time coordinate. The averaging is, of course, also over an unperturbed ensemble with density matrix ρ_0.

Recollecting the definition (3.2) of the retarded Green function, we get from (14.5)

$$\begin{aligned}\tilde{C}_2(x_0) &= \tilde{C}_2^{(0)}(x_0) \\ &\quad + \int_{-\infty}^{+\infty} dx_0'\, A_m\, e^{-i\omega x_0'}\,\theta(x_0-x_0')\langle [C_2(x_0), C_1(x_0')]_- \rangle\, e^{-\varepsilon|x_0|} \\ &= \tilde{C}_2^{(0)}(x_0) + \int_{-\infty}^{+\infty} dx_0'\, A_m\, e^{-i\omega x_0'} \ll C_2(x_0)\,|\,C_1(x_0') \gg_r^{(-)} . \quad (14.6)\end{aligned}$$

As the Green function $\ll C_2(x_0)\,|\,C_1(x_0') \gg_r^{(-)} \equiv K_{21,r}^{(-)}(x_0, x_0')$ is inevitably damped, if we take dissipative processes into account, we can at once put $\varepsilon = 0$. Moreover, writing

$$\frac{1}{2\pi}\int_{-\infty}^{+\infty} dt\, e^{iEt}\, K_{21,r}^{(-)}(x_0, x_0') = K_{21,r}^{(-)}(E) , \quad (14.7)$$

we find

$$\tilde{C}_2(x_0) = \tilde{C}_2^{(0)}(x_0) + \chi(\omega)\, A_m\, e^{-i\omega x_0} . \quad (14.8)$$

Here we have

$$\chi(\omega) = i\int_{-\infty}^{+\infty} dt\ \theta(t)\langle [C_2(x_0), C_1(x_0')]_- \rangle\, e^{i\omega t} , \quad (14.9)$$

that is,

$$\chi(\omega) = 2\pi\, K_{21,r}^{(-)}(E)\Big|_{E=\omega} . \quad (14.10)$$

The quantity $\chi(\omega)$ is sometimes called the complex admittance of the system. Using (3.7) and (2.11) we can easily immediately express $\chi(\omega)$ in terms of the spectral functions corresponding to the commutator or the anticommutator of C_2 and C_1:

$$\chi(\omega) = \int_{-\infty}^{+\infty} dE \, \frac{J_{21}^{(-)}(E)}{E - \omega - i\varepsilon} = \int_{-\infty}^{+\infty} dE \, \frac{\tanh \frac{\beta E}{2} J_{21}^{(+)}(E)}{E - \omega - i\varepsilon} . \quad (14.11)$$

The quantities describing the reaction of the system (and in particular also the absorption of energy by the system) to an arbitrary external perturbation can thus immediately be expressed in terms of the time-correlation functions for the corresponding operators C_1 and C_2.

The case $C_1 = C_2$ is of special interest. The correlation function

$$K^{(+)}(t) = \int_{-\infty}^{+\infty} dE \, e^{-iEt} J^{(+)}(E)$$

describes then the evolution in time of the spontaneous fluctuations of the quantity described by the operator $C_2(x_0)$ under thermodynamic equilibrium conditions. Through (14.8) and (14.9) it also describes ultimately the dissipation of the energy of the external field in the system considered. This fact is really the contents of the so-called "fluctuation-dissipation theorem" (Callen and Welton 1951).

In applications one is usually interested in the case where C_2 is Hermitean (C_1,is, of course, always Hermitean). We have then clearly $J^{(+)}(E) = J^{(+)+}(-E)$ and one sees easily from (14.11) that we have for the admittance:

$$\text{Re } \chi(\omega) = \text{Re } \chi(-\omega) , \quad (14.12)$$

$$\text{Im } \chi(\omega) = - \text{Im } \chi(-\omega) . \quad (14.13)$$

If, moreover, the spectral function turns out to be real, the dispersion relations of section 4 are valid for $K_{21,r}^{(+)}(\lambda)$. Separating in (14.11) the real and the imaginary parts we get in this case

$$\text{Re } \chi(\omega) = \int_{-\infty}^{+\infty} dE \, \tanh \frac{\beta E}{2} \, \mathcal{P} \frac{J_{21}^{(+)}(E)}{E - \omega} , \quad (14.14)$$

$$\text{Im } \chi(\omega) = \pi \tanh \frac{\beta\omega}{2} J_{21}^{(+)}(\omega) , \quad (14.15)$$

$$\text{Re } \chi(\omega) = \frac{1}{\pi} \int_{-\infty}^{+\infty} dE \, \mathcal{P} \frac{\text{Im } \chi(E)}{E - \omega} , \quad (14.16)$$

$$\text{Im } \chi(\omega) = - \int_{-\infty}^{+\infty} dE \, \mathcal{P} \frac{\text{Re } \chi(E)}{E - \omega} \quad (14.16a)$$

As was the case for the dispersion relations of section 4, (14.16) and (14.16a) have been written down, under the assumption that Im $\chi(E)$ decreases sufficiently fast with increasing $|E|$ and that the integral converges. (Such a situation is just typical for statistical mechanics problems.) If this condition were not satisfied we should have re-

course to the procedures developed in connexion with quantum field theory problems (Bogolyubov, Medvedev, and Polivanov 1958; in the simplest case this would lead to the occurrence of the difference Im $\chi(E)$ - Im $\chi(\omega)$ in (14.16)).

Equations (14.9) and (14.10) describe the reaction of the system to the external perturbation of arbitrary physical nature; the only requirement is that the corresponding interaction Hamiltonian can be written in the form (14.1). We shall specialise these expressions now for two important particular cases referring to systems in uniform magnetic or in uniform electrical fields.

Let, to begin with,

$$\Delta H = - M_i \mathcal{H}_i(x_0) , \tag{14.17}$$

where M_i is the magnetic moment per unit volume and $\mathcal{H} = \mathcal{H}_m e^{-i\omega x_0}$ is the field strength of the external magnetic field. It is clear that in this case the vector $\vec{M}$ plays the role of the operator C_1; it is, however, also the operator C_2 as we are interested in the average magnetisation in the sample. The admittance $\chi(\omega)$ is in this case nothing but the complex magnetic susceptibility tensor $\chi_{ij}(\omega)$. Since the magnetic moment is an additive operator,

$$M_i(x_0) = \int d\lambda \, d\lambda' \, (\lambda | M_i | \lambda') \, a^+(\lambda, x_0) \, a(\lambda', x_0) ,$$

(14.10) gives an expression for $\chi_{ij}(\omega)$ in terms of two-particle Green functions of the kind (5.24):

$$\chi_{ij}(\omega) = 2\pi \int d\lambda_1 \, d\lambda_2 \, d\lambda_1' \, d\lambda_2' (\lambda_2 | M_j | \lambda_2')(\lambda_1 | M_i | \lambda_1') \, G^{(-)}_{2,r}(\lambda_1, \lambda_1'; \lambda_2, \lambda_2'; \omega) , \tag{14.18}$$

$$G^{(-)}_{2,r}(\lambda_1, \lambda_1'; \lambda_2, \lambda_2'; E) = \frac{i}{2\pi} \int_{-\infty}^{+\infty} dt \, \theta(t) \, \langle [a^+(\lambda_1, x_0) \, a(\lambda_1', x_0), a^+(\lambda_2, x_0') \, a(\lambda_2', x_0')]_- \rangle \, e^{iEt} . \tag{14.19}$$

The spectral function is in this case clearly real, and (14.16) and (14.16a) are thus valid, as well as the dispersion relations connecting the real and the imaginary parts of the magnetic susceptibility.

We turn now to the second particular case where a system is in a uniform electrical field of strength $\mathcal{E} = \mathcal{E}_m e^{-i\omega x_0 - \varepsilon |x_0|}$. The Hamiltonian (14.1) is then given by

$$\Delta H = - (\mathcal{E}_m \cdot \vec{d}(x_0)) \, e^{-i\omega x_0 - \varepsilon |x_0|} , \tag{14.20}$$

where $\vec{d}$ is the total dipole moment of the system. It is clear that it plays the role of the operator C_1; the averaged operator C_2 is here the current density $\vec{j}$. The function $\chi(\omega)$ is in this case the complex electrical conductivity tensor which we denote by $\sigma_{il}(\omega)$. Equation

(14.16a) becomes then the well-known Kramers-Kronig dispersion relation (Kronig 1926, Kramers 1927) connecting the real and the imaginary parts of the dielectric constant ϵ. Indeed, the electrical conductivity and the dielectric tensors are connected by the well-known relations

$$\text{Im } \sigma_{ij}(\omega) = -\omega \text{ Re } \epsilon_{ij}(\omega) , \qquad \text{Re } \sigma_{ij}(\omega) = \omega \text{ Im } \epsilon_{ij}(\omega) . \tag{14.21}$$

Substituting (14.21) into (14.16a), using (14.13), and noting that as $\omega \to \infty$, Re $\epsilon_{ij}(\omega) \to \delta_{ij}$, we find easily

$$\text{Re } \epsilon_{ij}(\omega) - \delta_{ij} = \frac{1}{\pi} \int_{-\infty}^{+\infty} dE \, \mathcal{P} \, \frac{\text{Im } \epsilon_{ij}(E)}{E - \omega} , \tag{14.22}$$

which is the Kramers-Kronig relation in tensor form.

From (14.9) we get in this case

$$\sigma_{il}(\omega) = i \int_{-\infty}^{+\infty} dt \; \theta(t) \, \langle [j_i(x_0), d_l(x_0')]_- \rangle \, e^{i\omega t} . \tag{14.23}$$

Integrating by parts we get

$$\sigma_{il}(\omega) = -\frac{1}{\omega} \int_{-\infty}^{+\infty} dt \; e^{i\omega t} \, \{ \delta(t) \, \langle [j_i(x_0), d_l(x_0')]_- \rangle - \theta(t) \, \langle [j_i(x_0), \frac{\partial}{\partial x_0'} d_l(x_0')]_- \rangle \} . \tag{14.24}$$

The commutator in the first term need only be evaluated for $x_0 = x_0'$. We restrict ourselves here as in section 13 to spatially uniform systems. Bearing in mind possible applications to solid state theory we can not yet write the kinetic operator in the form $T(\vec{p}) = \vec{p}^2/2m_0$, and we have thus for the velocity $\vec{v}(\vec{p}) = \nabla_{\vec{p}} T(\vec{p}) \neq \vec{p}/m_0$ (see the discussion following (13.24)). Denoting, as in section 13, the result of averaging $\vec{v}$ over different directions over a $T(\vec{p})$ = constant-surface by $\vec{p} f(\vec{p}^2)$ we find easily

$$\langle [j_i(x_0), d_l(x_0)]_- \rangle = -ine^2 \sum_{\vec{p}} n(\vec{p}) \, \{ \delta_{il} \, f(\vec{p}^2) + 2 \, p_i \, p_l \, f'(\vec{p}^2) \} . \tag{14.25}$$

The dash on f indicates here differentiation with respect to its argument, and $n(\vec{p})$ is the distribution function, normalised per unit volume. In accordance with what we said earlier in this section, $n(\vec{p})$ must be evaluated for the case where there is no field $\mathcal{E}$, that is, under equilibrium conditions. We have then $n(\vec{p}) = n(-\vec{p})$ and the right-hand side of (14.25) is thus proportional to the unit tensor. Writing

$$\sum_{\vec{p}} n(\vec{p}) \, \{ f(\vec{p}^2) + \frac{2}{3} \, \vec{p}^2 \, f'(\vec{p}^2) \} = \frac{1}{\tilde{m}} , \tag{14.26}$$

we get

$$\langle [j_i(x_0), d_l(x_0)]_- \rangle = -\frac{ine^2}{\tilde{m}} \, \delta_{il} . \tag{14.27}$$

We can call $\tilde{m}$ the average effective mass. In particular, if $T(\vec{p})$ is given by (13.25), $\tilde{m}$ becomes the effective mass m^* of (13.27).

The generalisation of (14.27) to the case when there are several kinds of charged particles is, as in section 13, easily done and reduces to substituting $\Sigma_a(n_a e_a^2/m_a)$ for ne^2/m, where the index a again enumerates the different kinds of particles and where the summation is over all those kinds.

Moreover, we have

$$\frac{\partial}{\partial x_0'} d_l(x_0') = \int d^3\vec{x}'\, j_l(x') \,.$$

We finally get thus

$$\sigma_{il}(\omega) = \frac{ine^2}{\tilde{m}\omega}\,\delta_{il} + \frac{1}{\omega}\int_{-\infty}^{+\infty} dt\, d^3\vec{x}'\, e^{i\omega t}\,\theta(t)\,\langle [j_i(x), j_l(x')]_- \rangle \,. \qquad (14.28)$$

As the current density is an additive operator, we can use (14.10) and directly express σ_{il} in terms of the two-particle Green function (14.19). We can use (14.18) and put in that equation $\lambda = \{\vec{x}, s\}$ and replace the matrix elements of the magnetic moment by the matrix elements of the current density.

Some times it may, however, turn out to be more convenient to consider "current fields" and identify $j_i(x)$ and $j_l(x')$ with the "primary" operators C_1 and C_2 in the general formulae of section 4.

The electrical conductivity tensor can then easily be expressed in terms of the current correlation function (13.15). Indeed, if we put

$$\langle [j_i(x), j_l(x')]_- \rangle = \int_{-\infty}^{+\infty} dE\, e^{-iEt}\, F_{il}^{(-)}(\vec{x}, \vec{x}'; E) \qquad (14.29)$$

and use (2.10), we get

$$\begin{aligned}
\sigma_{il}(\omega) &= \frac{ine^2}{\tilde{m}\omega}\,\delta_{il} + \frac{1}{\omega}\int_{-\infty}^{+\infty} dt \int d^3\vec{x}'\, e^{i\omega t}\,\theta(t) \int_{-\infty}^{+\infty} dE\, e^{-iEt}\, F_{il}^{(-)}(\vec{x}, \vec{x}'; E) \\
&= \frac{ine^2}{\tilde{m}\omega}\,\delta_{il} - \frac{i}{\omega}\int_{-\infty}^{+\infty} dE \int d^3\vec{x}'\, \frac{F_{il}^{(-)}(\vec{x}, \vec{x}'; E)}{E - \omega - i\varepsilon} \\
&= \frac{ine^2}{\tilde{m}\omega}\,\delta_{il} - \frac{i}{\omega}\int_{-\infty}^{+\infty} dE\, \frac{\tanh \frac{1}{2}\beta E}{E - \omega - i\varepsilon} \int d^3\vec{x}'\, F_{il}^{(+)}(\vec{x}, \vec{x}'; E) \,. \qquad (14.30)
\end{aligned}$$

In the case of a spatially uniform system which is of interest to us $F^{(+)}(\vec{x}, \vec{x}'; E)$ is given by (13.15) to (13.19); we get thus from (14.30)

$$\begin{aligned}
\sigma_{il}(\omega) = \frac{ine^2}{\tilde{m}\omega}\,\delta_{il} &- \frac{i}{\omega}(2\pi)^3 \int_{-\infty}^{+\infty} dE\, \mathcal{P}\, \frac{\tanh \dfrac{\beta E}{2}}{E - \omega}\, F_{il}^{(+)}(0, E) \\
&+ (2\pi)^3\, \frac{\pi \tanh \dfrac{\beta\omega}{2}}{\omega}\, F_{il}^{(+)}(0, \omega) \,. \qquad (14.31)
\end{aligned}$$

As should have been expected, the current in a uniform field (and in a uniform medium) is determined solely by the Fourier components of the correlation function at $\vec{k} = 0$. It follows from (13.19) that under those conditions $F_{il}^{(+)}$ reduces simply to F_1: $F_{il}^{(+)}(0,E) = \delta_{il} F_1(0,E^2)$. The electrical conductivity tensor reduces thus to a scalar, σ (as should be the case in a medium with this symmetry); its real part is positive (see (13.20)). From (14.31) we have

$$\text{Re } \sigma(\omega) = (2\pi)^3 \frac{\pi \tanh \frac{\beta\omega}{2}}{\omega} F_1(0,\omega^2) = \text{Re } \sigma(-\omega) . \qquad (14.32)$$

The static electrical conductivity, in particular, is given by

$$\text{Re } \sigma(0) = \frac{\pi\beta}{2} (2\pi)^3 F_1(0,0) . \qquad (14.33)$$

For the imaginary part of σ we get

$$\text{Im } \sigma(\omega) = \frac{ne^2}{\tilde{m}\omega} - \frac{(2\pi)^3}{\omega} \int_{-\infty}^{+\infty} dE \, \mathcal{P} \frac{F_1(0,E^2)}{E - \omega} \tanh \frac{\beta E}{2} = -\text{Im } \sigma(-\omega) . \qquad (14.34)$$

We can rewrite this equation also in the form

$$\text{Im } \sigma(\omega) = \frac{ne^2}{\tilde{m}\omega} - (2\pi)^3 \int_{-\infty}^{+\infty} dE \frac{\tanh \frac{\beta E}{2}}{E} \mathcal{P} \frac{F_1(0,E^2)}{E - \omega} . \qquad (14.34a)$$

From (14.31) and (14.34) there follow immediately several general statements.

First of all, we can neglect the second term on the right-hand side of (14.34) in the limit of very high frequencies. We have then

$$\text{Im } \sigma(\omega) = \frac{ne^2}{\tilde{m}\omega} ,$$

and thus

$$\text{Re } \varepsilon(\omega) = 1 - \frac{ne^2}{\tilde{m}\omega^2} . \qquad (14.35)$$

At high frequencies the real part of the dielectric constant tends thus to the value which is characteristic for a system of free charges, provided we take for the mass the quantity $\tilde{m}$. In the case of charged particles in vacuo (when there is only an uniform spatial distribution of the compensating charge) this would be the true particle mass m_0. In solids, however, this would be a more complicated quantity. In particular, it may be temperature-dependent, according to (14.26).

Secondly, let us consider the integral of Re $\sigma(\omega)$ over all frequencies. Using (13.25) and the fact that $\sigma(\omega)$ is even, we get

$$\int_0^\infty \text{Re } \sigma(\omega) \, d\omega = \frac{\pi ne^2}{2} f(0) , \qquad (14.36)$$

where $f(\vec{k})$ was defined in section 13.

We call (14.36) a sum rule. If there were several kinds of current carriers, we would have on the right-hand side the sum $(\pi/2)\,\Sigma_a\, n_a\, e_a\, f_a(0)$.

Expression (14.32) takes on a very obvious form in the special case when the current correlation function is simply exponentially damped,

$$<[j_i(x),j_l(x')]+> = <[j_i(\vec{x},0),j_l(\vec{x}',0)]_+> e^{-\frac{|x_0-x_0'|}{\tau}}, \qquad (14.37)$$

where τ is a constant. It is clear that the corresponding spectral function is of the form $C/(1+E^2\,\tau^2)$, where C is independent of E. The approximation (14.37) means thus an assumption about the purely imaginary poles of the spectral function. We get then for the real part of the electrical conductivity tensor

$$\mathrm{Re}\;\sigma(\omega) = 2\pi\frac{\tanh\frac{\beta\omega}{2}}{\omega}\int d^3(\vec{x}-\vec{x}')<[j_i(\vec{x},0),j_l(\vec{x}',0)]_+>\frac{\tau}{1+\omega^2\,\tau^2}\,. \qquad (14.38)$$

We can in this case interpret τ as the mean free time of flight. If we neglect quantum corrections ($[\tanh\frac{1}{2}\,\beta\omega]/\omega \to \beta/2$) the frequency-dependence of (14.38) is the one well known from the usual transport theory. We emphasise, however, that it is not known in advance whether one can write the correlation function in the simple form (14.37).

15. THE REACTION OF A SYSTEM TO EXTERNAL ACTION; REPRESENTATION THROUGH THE VERTEX PART *

When we wish to apply the theory of the preceding section to specific problems we need first evaluate the two-particle (or even more complicated) Green functions. This reduces as a rule to solving equations such as the transport equation, that is, to a fairly complicated problem. For this reason it is very desirable to get another expression for the transport coefficients in which other kinds of functions occur. One such possibility will be considered in the present section. Of course, also here we must expect to obtain expressions which are only formally compact and which contain quantities which are in fact unknown. In some cases, however, it may turn out to be more convenient to evaluate just those quantities rather than the two-particle Green functions.

To fix our ideas we shall consider the electrical conductivity tensor under such conditions that Ohm's law is valid; from the derivations it will, however, be clear that the method developed here is equally suitable to evaluate any transport coefficients.

* Bonch-Bruevich 1959c.

The conductivity current density operator in an external field with four-potential $\tilde{A}_\beta = \{\tilde{A}_0, \tilde{\vec{A}}\}$ is of the form

$$j_i(x) = \frac{ie}{2m}\left(\frac{\partial\psi^+}{\partial x_i}\psi - \psi^+\frac{\partial\psi}{\partial x_i}\right) - \frac{e^2}{2mc_0}\tilde{A}_i(x)\,\psi^+(x)\,\psi(x)\,. \qquad (15.1)$$

We have thus for the average current density

$$\tilde{j}_i(x) = \tilde{j}_i^{(1)}(x) + \tilde{j}_i^{(2)}(x)\,, \qquad (15.2)$$

where we have from (5.5)

$$\tilde{j}_i^{(1)}(x) = \frac{e}{2m}\lim_{\substack{x'\to x\\ x_0'>x_0}}\left(\frac{\partial}{\partial x_i} - \frac{\partial}{\partial x_i'}\right)\mathrm{Tr}\;G_c(x, x'; A)\,, \qquad (15.3)$$

$$\tilde{j}_i^{(2)}(x) = -\frac{ie^2}{2mc_0}\tilde{A}_i(x)\lim_{\substack{x'\to x\\ x_0'>x_0}}\mathrm{Tr}\;G_c(x, x'; A)\,. \qquad (15.4)$$

Here $G_c(x, x'; A)$ is the single-particle causal Green function, evaluated taking into account the external electromagnetic field (this is indicated by the functional argument A) and also the interaction causing the damping. As we are only interested in effects linear in the external field, we can use the definition (9.4a) of the vertex part, and write

$$G_c(x, x'; A) = G_c(x, x') + e\int d^4y\,\frac{\delta G_c(x, x'; A)}{\delta e\tilde{A}_\beta(y)}\,\tilde{A}_\beta(y)$$

$$= G_c(x, x') + e\int d^4y\,d^4y'\,d^4y''\;G_c(x, y')\,\Gamma_e^\beta(y', y''; y)\,G_c(y'', x')\,\tilde{A}_\beta(y)\,, \qquad (15.5)$$

where

$$\Gamma_e^\beta(y', y''; y) = -\frac{\delta G_c^{-1}(y', y'')}{\delta e\tilde{A}_\beta(y)} \qquad (15.6)$$

is the "electromagnetic" vertex part and $G_c(x,x')$ the Green function for the system without the electromagnetic field. In general, one must choose the limits of the integration in (15.5) taking the causality condition into account. In order to avoid computational complications which are connected with this we shall consider only the limiting case $x_0 \to \infty$. We shall not mention this explicitly in the following, but it will be understood to be the case.

When there is no external field, the average current in the system will, in general, be equal to zero *. The first term on the right-

* Superconductors are an exception. The electrical conductivity tensor is,

hand side of (15.5) does therefore not contribute to $\tilde{j}_i^{(1)}(x)$. On the other hand, only this term should be substituted into $\tilde{j}_i^{(2)}$ in the linear approximation. Combining (15.2) to (15.5) we get thus

$$\tilde{j}_i(x) = \int \lambda_i^{\beta}(x, y)\, \tilde{A}_{\beta}(y)\, d^4y\,, \tag{15.7}$$

where

$$\lambda_i^{\beta}(x, y) = \frac{e^2}{2m} \lim_{\substack{x' \to x \\ x_0' < x_0}} \left(\frac{\partial}{\partial x_i} - \frac{\partial}{\partial x_i'}\right) \mathrm{Tr} \int d^4y'\, d^4y''\, G_c(x, y')$$

$$\times\, \Gamma_e^{\beta}(y', y''; y)\, G_c(y'', x')$$

$$- \frac{ie^2}{2mc_0} \lim_{\substack{x' \to x \\ x_0' > x_0}} \mathrm{Tr}\, G_c(x, x')\, \delta(x-y)\, \delta_{i\beta}\,. \tag{15.8}$$

We now compare (15.8) and (9.13). Since in the non-relativistic limit $\gamma_i \to v_i/c$, we see that the right-hand side of (15.8) reduces simply to $\mathcal{P}_i^{\beta}$.

The quantities λ_i^{β} are connected with the electrical conductivity tensor σ_i^j. Indeed, by definition

$$j_i(x) = \int \sigma_i^j(x, y)\, \mathcal{E}_j(y)\, d^4y\,, \tag{15.9}$$

where $\mathcal{E}_j(y)$ is the strength of the external electrical field which is connected with the four-potential by the relation

$$\mathcal{E}_j(y) = \frac{\partial \tilde{A}_0(y)}{\partial y_j} - \frac{1}{c_0} \frac{\partial \tilde{A}_j(y)}{\partial y_0}\,. \tag{15.10}$$

From (15.7), (15.9), and (15.10) we get

$$\lambda_i^j(x, y) = \frac{1}{c_0} \frac{\partial \sigma_i^j(x, y)}{\partial y_0}\,, \qquad \lambda_i^0(x, y) = -\frac{\partial \sigma_i^j(x, y)}{\partial y_j}\,. \tag{15.11}$$

In the following we shall restrict ourselves to the case of spatially uniform systems and no external force field, and we shall take the potential $\tilde{A}_{\beta}(y)$ to be of the form *

$$\tilde{A}_{\beta}(y) = \tilde{A}_{\beta}(k)\, e^{-iky}\,. \tag{15.12}$$

however, always without exception determined only by that part of the current which tends to zero together with the field; the following formulae are thus always applicable.

* To take in account the adiabatic switching on and off of the interaction at $y_0 \to \pm\infty$, it would be sufficient to introduce a fictitious damping by giving k_0 an infinitesimally small imaginary part of appropriate sign. In actual fact, this is unnecessary as in systems with a finite electrical conductivity there is always also a finite damping present.

It is clear that then the current density can also be written in similar form:

$$\tilde{j}_i(x) = \tilde{j}_i(k)\, e^{-ikx}\,, \tag{15.13}$$

and we get from (15.7), (15.8), and (15.11)

$$\tilde{j}_i(k) = \lambda_i^{\beta}(k)\, \tilde{A}_{\beta}(k)\,, \tag{15.14}$$

$$\lambda_i^{\beta}(k) = \frac{ie^2}{m}(2\pi)^4 \lim_{t\to+0} \int_{-\infty}^{+\infty} dp_0\, e^{ip_0 t}\, \mathrm{Tr} \int d^3\vec{p}\; p_i\, G_c(p+\frac{k}{2})$$

$$\times\, \Gamma_e^{\beta}(p+\frac{k}{2}, p-\frac{k}{2})\, G_c(p-\frac{k}{2})$$

$$-\frac{ie^2}{2mc_0} \lim_{t\to+0} \mathrm{Tr} \int_{-\infty}^{+\infty} dp_0\, e^{ip_0 t} \int d^3\vec{p}\; G_c(p)\,, \tag{15.15}$$

$$i\,\sigma_i^j\, k_j = \lambda_i^0\,, \qquad i\,\sigma_i^j\, k_0 = c_0\, \lambda_i^j\,. \tag{15.16}$$

The Fourier transform of the vertex part is here defined by the equation

$$\Gamma_e^{\beta}(y', y''; y) = \frac{1}{(2\pi)^8} \int d^4q'\, d^4q''\, e^{-i(q', y'-y)+i(q'', y''-y)}\, \Gamma_e^{\beta}(q', q'')\,.$$

Equations (15.15) and (15.16) determine the electrical conductivity tensor, taking both the time- and the spatial dispersion fully into account. When we use them we must bear in mind one important fact, namely, that when expressing in (15.5) the functional derivative $\delta G_c/\delta e\tilde{A}_{\beta}$ in terms of the vertex part, we should multiply by G_c. This operation is, however, in general a singular one, and the formulae obtained may thus turn out to be non-unique. To remove this lack of uniqueness we must take into account the general properties of the electrical conductivity tensor as function of the complex variable k_0. We know (see the preceding section) that this function is analytical in the upper half-plane. When in doubt, we must thus consider k_0 as a complex variable with a positive imaginary part $\mathrm{Im}\, k_0 = \gamma > 0$, and only in the final result take the limit $\gamma \to 0$ (the same result is, of course, also obtained if we take into account the adiabatic switching on of the interaction at $y_0 \to -\infty$).

We consider, in particular, a system of charged particles in an external field which is sufficiently slowly varying in time and in space. The first condition allows us to put the vector potential equal to zero (formally we can take the limit $c_0 \to \infty$) and as a result the last term on the right-hand side of (15.15) disappears; because of the second condition only the lowest powers in $\vec{k}$ can remain in (15.15). We find then easily

$$\sigma_i^j(k_0) = \frac{e^2}{m}(2\pi)^4 \,\mathrm{Tr}\,\frac{\partial}{\partial k_j}\int d^3\vec{p}\; p_i \times \lim_{t\to+0}\int_{-\infty}^{+\infty} dp_0\, e^{ip_0 t}\, G_c(p+\tfrac{k}{2})\,\Gamma_e^0(p+\tfrac{k}{2}, p-\tfrac{k}{2})\, G_c(p-\tfrac{k}{2})\Big|_{k=0} \quad (15.17)$$

We note that by definition the quantity m in (15.1), and thus in (15.17), is the true mass of the charged particle. If we wish to use the results obtained here in solid state theory and if we wish to restrict ourselves at the same time to considering only spatially uniform systems we must (as in previous sections) perform the substitution

$$\frac{p_i}{m} \to v_i(\vec{p}) = \frac{\partial W(\vec{p})}{\partial p_i}\,, \quad (15.18)$$

where $W(\vec{p})$ is the electron energy as a function of its quasi-momentum $\vec{p}$.

As an illustration we shall consider the case of a free electron gas. We have then for G_c (see (5.20))

$$G_c(p) = -\frac{1}{(2\pi)^4}\frac{p_0 - W(\vec{p}) + i\eta[2n_F(\vec{p})-1]}{[p_0 - W(\vec{p})]^2 + \eta^2}\,,$$

$$\eta \to +0\,, \qquad W(\vec{p}) = \frac{\vec{p}^2}{2m}\,, \qquad \Gamma_e^0 = 1\,.$$

Hence

$$\mathrm{Tr}\lim_{t\to+0}\int_{-\infty}^{+\infty} dp_0\, e^{ip_0 t}\, G_c(p+\tfrac{k}{2})\, G_c(p-\tfrac{k}{2}) = \frac{2i}{(2\pi)^7}\left\{\frac{n_F(\vec{p}+\frac{\vec{k}}{2})}{-k_0 + W(\vec{p}+\frac{\vec{k}}{2}) - W(\vec{p}-\frac{\vec{k}}{2})} + \frac{n_F(\vec{p}-\frac{\vec{k}}{2})}{k_0 - W(\vec{p}+\frac{\vec{k}}{2}) + W(\vec{p}-\frac{\vec{k}}{2})}\right\}. \quad (15.19)$$

In accordance with what we said a moment ago we must evaluate the integral of (15.19), considering k_0 to be a complex variable

$$k_0 = \omega + i\gamma\,, \qquad \gamma > 0\,. \quad (15.20)$$

Expanding in powers of $\vec{k}$ we get from (15.19) and (15.17)

$$\mathrm{Re}\,\sigma_i^j(\omega) = -\frac{e^2}{m^2}\cdot\frac{2}{(2\pi)^3}\cdot\delta_{ij}\int d^3\vec{p}\;\vec{p}^2\,\frac{\partial n_F(\vec{p})}{\partial W(\vec{p})}\,\frac{\gamma}{\omega^2+\gamma^2}\,, \quad (15.21)$$

$$\mathrm{Im}\,\sigma_i^j(\omega) = -\frac{e^2}{m}\,\frac{2}{(2\pi)^3}\int d^3\vec{p}\; p_i\, v_j\,\frac{\partial n_F(\vec{p})}{\partial W(\vec{p})}\,\frac{\omega}{\omega^2+\gamma^2}\,. \quad (15.22)$$

The right-hand side of (15.21) is formally the same as the result obtained by solving the transport equation, providing we identify γ^{-1} with the relaxation time. One should, however, not attach too much

importance to this fact: in our case γ is simply the imaginary part of the complex argument k_0. According to the condition of adiabatic switching on of the interaction, γ must be assumed to be infinitesimally small and the static conductivity (Re $\sigma_i^j(\omega)$ as $\omega \to 0$) diverges in that case, as should, of course, be the case in a system without damping. It is impossible to transfer immediately (15.21) and (15.22) to the case of a system with damping, as in that case the Green function does not have the simple form (5.20). Integrating (15.22) by parts, we get

$$\operatorname{Im} \sigma_i^j(\omega) = \frac{ne^2}{m\omega} \delta_{ij} , \tag{15.23}$$

where

$$n = \frac{2}{(2\pi)^3} \int d^3\vec{p}\, n_F(\vec{p})$$

is the total electron concentration. Using (14.21) we get from (15.23) the well-known expression for the dielectric susceptibility of a free electron gas

$$\varepsilon = 1 - \frac{ne^2}{m\omega^2} \tag{15.24}$$

(we remind the reader that we use Heaviside units for the charge).

Let us now turn to the general equation (15.17). We noted already at the beginning of this section that the functions G_c and Γ_e^0 occurring here refer to a system at equilibrium, and they may be assumed to be formally known if we consider transport problems. In actual fact one must determine the Green function from the equations of sections 9 and 10; on the other hand, the complete equations for the vertex part, as we shall now shew, can only be formulated approximately. We shall consider a system of charged particles interacting with a slowly varying classical external electromagnetic field and also with a quantised boson field characterised by a "potential" $\Phi(x)$ and a coupling constant g (this last interaction is just the one which causes relaxation processes and causes the electrical conductivity to be finite). We denote, as before, the causal Green function of that field by D_c, the mass operator describing the interaction of the electrons with the field by M, and the vertex part by Γ (to distinguish it from the "electromagnetic" vertex part Γ_e). We assume that we have solved the problem of the motion of electrons in the field Φ, that is, we assume that we know D_c and Γ. The equation of motion for $G_c(x, x')$ is in this case of the form (compare (9.7))

$$\left\{ i\frac{\partial}{\partial x_0} + \mu - T_{\vec{x}} - V(\vec{x}) + g\,\tilde{\Phi}(x) + e\tilde{A}_0 \right\} G_c(x, x') - \int d^4y\, M(x, y)\, G_c(y, x') = -\delta(x-x') . \tag{15.25}$$

We get thus from the definition (15.6)

$$\Gamma^{0}_{e}(y',y'';y) = \delta(y'-y'')\,\delta(y'-y) + g\frac{\delta\tilde{\Phi}(y')}{\delta e\tilde{A}_{0}(y)}\,\delta(y'-y'') - \frac{\delta M(y',y'')}{\delta e\tilde{A}_{0}(y)}. \quad (15.26)$$

It is convenient to use a symbolical notation for the evaluation of the functional derivatives. The average potential $\tilde{\Phi}$ is given by (10.3a)

$$\tilde{\Phi} = - D^{\prime(0)}_{c}(J + igf\,\Gamma^{(0)}\,G_{c}) .$$

Taking the variation of this expression with respect to $\tilde{A}_{0}$ we get

$$\frac{\delta\tilde{\Phi}}{\delta e\tilde{A}_{0}} = - i\,g\,D^{(0)}_{c}\,f\,\Gamma^{(0)}\,G_{c}\,\Gamma^{0}_{e}\,G_{c} . \quad (15.27)$$

In the spatially uniform case, $D'_{c} = D_{c}$. Moreover, we have from (9.5)

$$M = - i\,g^{2}\,\Gamma^{(0)}\,G_{c}\,\Gamma\,D_{c} ,$$

and thus

$$\frac{\delta M}{\delta e\tilde{A}_{0}} = - i\,g^{2}\,\Gamma^{(0)}\,\{G_{c}\,\Gamma^{0}_{e}\,G_{c}\,\Gamma\,D_{c} - G_{c}\frac{\delta\Gamma}{\delta e\tilde{A}_{0}}\,D_{c} - G_{c}\,\Gamma\frac{\delta D_{c}}{\delta e\tilde{A}_{0}}\}. \quad (15.28)$$

From the definition (9.4) of the vertex part we have

$$- \frac{\delta\Gamma}{\delta e\tilde{A}_{0}} = \frac{\delta\Gamma^{0}_{e}}{\delta g\tilde{\Phi}}. \quad (15.29)$$

To evaluate the functional derivative of D_{c} we write it in the form

$$\frac{\delta D_{c}}{\delta e\tilde{A}_{0}} = - D_{c}\frac{\delta D^{-1}_{c}}{\delta e\tilde{A}_{0}}\,D_{c} , \quad (15.30)$$

and we use (10.2b),

$$D^{-1}_{c} = [D^{(0)}_{c}]^{-1} - \mathcal{P} ,$$

where we have

$$\mathcal{P} = - i\,g^{2}\,\Gamma^{(0)}\,G_{c}\,\Gamma\,G_{c} .$$

We have thus

$$\frac{\delta D_{c}}{\delta e\tilde{A}_{0}} = - i\,g^{2}\,D_{c}\,\Gamma^{(0)}\,G_{c}\,\{\Gamma^{0}_{e}\,G_{c}\,\Gamma + \frac{\delta\Gamma}{\delta e\tilde{A}_{0}} + \Gamma\,G_{c}\,\Gamma^{0}_{e}\}\,G_{c}\,D_{c} . \quad (15.31)$$

Combining (15.26) to (15.31), we get

$$\Gamma^{0}_{e} = 1 - i\,g^{2}\,D^{(0)}_{c}\,f\,\Gamma^{(0)}\,G_{c}\,\Gamma^{0}_{e}\,G_{c} + i\,g^{2}\,\Gamma^{(0)}\,\{G_{c}\,\Gamma^{0}_{e}\,D_{c}\,\Gamma\,D_{c} + G_{c}\frac{\delta\Gamma^{0}_{e}}{\delta g\tilde{\Phi}}\,D_{c}$$
$$+ i g^{2}\,G_{c}\,\Gamma\,D_{c}\,\Gamma^{(0)}\,G_{c}\,[\Gamma^{0}_{e}\,G_{c}\,\Gamma - \frac{\delta\Gamma^{0}_{e}}{\delta g\tilde{\Phi}} + \Gamma\,G_{c}\,\Gamma^{0}_{e}]\,G_{c}\,D_{c}\} . \quad (15.32)$$

All quantities on the right-hand side of (15.32) must be evaluated for a system without an external electromagnetic field. The presence of functional derivatives of Γ^0_e indicates that in fact we are dealing here with an infinite set of equations. We can only break this set off if we use some kind of approximation. In particular, if the interaction of the charged particles with the quantum field Φ is sufficiently small we can retain only terms of lowest order in g^2. We find then a closed linear integral equation for Γ^0_e (written here in the momentum representation):

$$\Gamma^0_e(p+\frac{k}{2},p-\frac{k}{2}) = 1 - i\,g^2\,(2\pi)^8 D_c^{(0)}(k)\int d^4k'\,G_c(k'+\frac{k}{2})\,\Gamma^0_e(k'+\frac{k}{2},k'-\frac{k}{2})\,G_c(k'-\frac{k}{2})$$
$$+ i\,g^2\,(2\pi)^8\int d^4k'\,D_c(k')\,G_c(k'+p+\frac{k}{2})\,\Gamma^0_e(k'+p+\frac{k}{2},k'+p-\frac{k}{2})\,G_c(k'+p-\frac{k}{2})\,. \qquad (15.33)$$

One can only in some special cases obtain a solution of this equation in an explicit form.

16. QUASI-PARTICLES

The equations obtained in the preceding three sections are far from the final ones, notwithstanding their apparent simplicity: if we wish to apply them to an actual problem we must beforehand evaluate some of the Green functions and that can usually only be done approximately, as we have already mentioned. It is, however, very characteristic for the method given here that it is possible to derive a number of qualitative conclusions of a general character which are valid, independent of any approximation. In the present section we shall apply the relations obtained earlier to study the general problem of the elementary excitations of a many-body system. The question of elementary excitations ("quasi-particles") is one of the central problems of present-day theories of condensed media. The general statement has often been made (see, for instance, Landau and Lifshits 1951) that the low-lying excited states of any quantum system of interacting particles can be considered to be states of a perfect (or almost perfect) gas of some kind of elementary excitations ("quasi-particles"). Since this gas behaves like a system of free particles one obtains at once a clarification of the success of, for instance, the "free electron" theory of solids (see Vonsovskiĭ 1952, Bonch-Bruevich 1955b). If one postulates the existence of some kind of quasi-particle spectrum, one can apparently successfully explain a whole number of greatly varying phenomena. In those cases where it turned out to be possible to obtain an approximate solution of the dynamical problem of a particular many-body system, the elementary excitations hypothesis has, indeed, been corroborated. Nobody

has, however, up to now given a general basis for this hypothesis, and also nobody knows exactly the limits of its applicability. The Green function method enables us to make this problem a bit clearer.

We noted earlier that the fact itself of the existence of a "single-quasi-particle" spectrum of excited states follows immediately from the general spectral theorems of sections 3 to 5 which connect the energy spectrum of a system with the singularities of the single- and two-particle Green functions (see the discussion of (5.1), (5.25), (9.18), and (9.19)). In this sense the concept of elementary excitations is exactly based, without any approximations. One must, however, bear in mind that one aspect of the "single-quasi-particle" character of the spectrum can by itself not give a complete foundation for the elementary excitations hypothesis in the form in which it is usually employed. We still need to shew that the thermodynamic quantities connected with a given branch of the energy spectrum can be evaluated, by using the theory of a perfect gas. We saw in sections 9 and 12 that, provided bilinear expansions such as (9.26) are applicable, this is, indeed, the case (see (9.31), (9.33), and (12.38)).

The average energy of a system of interacting particles is thus written as a sum of average energies of perfect gases of quasi-particles; the energy levels of these quasi-particles are determined by the eigenvalues of the effective wave equations for $G_c(\vec{x}, \vec{x}'; E)$ and $G_{2,c}(\vec{x}, \vec{x}'; E)$; the quantities $Z'(E, v)$ and $Z_2'(E', v')$ play here the role of the densities of state per unit volume in the intervals $dE\, dv$ and $dE'\, dv'$, respectively. It is important to note that - even in a system of fermions - one of these gases is a boson gas (the second term in (12.38)).

This means that in a fermion system one can distinguish at least two branches of the excitation spectrum: a fermion * and a boson branch. It is, of course, possible that there are several fermion branches or several boson branches. This happens, for instance, if the eigenvalues of the corresponding effective wave equations form several (possibly overlapping) different groups.

In this connexion we make a few remarks.

First of all, we note that bilinear expansions such as (9.26) are not exact. We noted in section 9 that they are only valid, if we can neglect the imaginary parts of the eigenvalues of equations such as (9.18), that is, if we neglect the damping of the corresponding excitations. In other words, the idea of describing the excited states of a system in terms of a quasi-particle gas is valid only inasmuch as the quasi-stationary states of such a gas may simply be considered to be stationary. In that sense the idea of elementary excitations is an approximate one; one can only use it as long as the "line width" is small compared to the excitation energy per particle.

* The fermion branch excitations are usually called charge-carriers, or current-carriers, if they are electrically charged.

Secondly, we noted in section 9 that (9.31) and (9.33) only permit us to use the equations of a perfect gas to evaluate additive thermodynamic quantities. When we wish to evaluate averages of binary (or even more complicated) operators, we need to know higher order density matrices, ρ_2 and so on, which are connected with Green functions of corresponding order. We saw that these can also be written in the form of an expansion such as (9.26) under certain well-defined conditions; the eigenfunctions and eigenvalues occurring in these expansions will, however, in general be different from the ones occurring in the expression for G_c. This means that different quasi-particle gases may correspond to different kinds of thermodynamic quantities (such as additive, binary, ... quantities). One should also bear in mind that the conditions for the applicability of bilinear expansions for different Green functions are determined by different parameters which need to be small.

Thirdly, even when (9.26) is applicable, the so-called quasi-particle energies are far from being purely mechanical quantities: we noted several times that they are, generally speaking, temperature-dependent. In other words, the characteristics of the quasi-particle spectrum are thermodynamic quantities. This fact leads to a number of consequences which so far have not yet been studied to any large extent.

Chapter IV

PLASMA OSCILLATIONS IN SOLIDS

17. STATEMENT OF THE PROBLEM

One of the most important applications of the methods developed in the preceding chapters is the single-electron theory of solids. We are here first of all concerned with taking the Coulomb interaction between the electrons consistently into account.

In a number of cases it is not necessary to do this explicitly - it is sufficient to stipulate simply the existence of elementary excitations *; there is, however, a whole class of important problems where an explicit dynamical consideration of the single-electron system is, apparently, inevitable. The problem of the basis of the elementary excitation method is relevant to a number of such problems. We saw in section 16 that the Green function method solves this problem in a general form.

If we wish to find out all possible kinds of elementary excitations in a given system, we need, however, an explicit solution of the Schrödinger equation for the given case. This is especially true for the theory of plasma oscillations which are apparently studied most naturally by Green function methods. Quantum corrections may turn out to be important in solids and this makes it somewhat risky to apply the standard Boltzmann transport equation method.

Moreover, a dynamical approach is necessary for the study of the influence of the different nature of structural defects on the electron energy specfrum in semi-conductors and metals. Finally, this approach is apparently necessary in problems concerning the exchange of energy between charge carriers and their environment in the crystal. The most important example of problems of this kind is the theory of carrier recombination in semi-conductors.

We must emphasise that a totally microscopic approach to the study of the electron energy spectrum in a solid is connected with extraordinary mathematical difficulties of a general nature, which are not characteristic of just the single-electron problem. These difficulties occur also in the usual "single-electron" theory and are connected with the necessity to solve the problem of the motion of

* This is, for instance, the case in the theory of galvanomagnetic phenomena in metals (see especially Lifshits, Azbel', and Kaganov 1956).

one electron in the periodic field of a perfect lattice. We are here speaking about the fact that it is natural to include among the electrons which determine the electrical, magnetic, ... properties of a solid only those from the outer one or two shells, but not those from all the shells. The specific division into "electrons" and "atomic cores" depends, of course, on the nature of the substance and the character of the problem considered (vide infra). However, even for an isolated atom it is usually impossible to give the electron density in a simple analytical form. As a result either must we appeal to more or less crude approximate methods or must deal with equations of unknown form. For this reason it is in general expedient to give up the idea of evaluating in all detail the electron spectrum in a perfect lattice, and to determine its parameters from experimental data. It is convenient, for instance, to use in semi-conductors for these data those on (diamagnetic) cyclotron resonance (Dorfman 1951, Dresselhaus, Kip, and Kittel 1955); in metals the use of galvanomagnetic data (Lifshits, Azbel', and Kaganov 1956) and the study of ultrasound absorption in a magnetic field (Gurevich 1959) promises to be successful. The dynamic theory must then answer the following problems:

a. How does the energy spectrum of the "free" particles change, if we take the interaction into account?
b. What new branches of the spectrum (as compared with a perfect gas) occur because of the interaction?
c. How is the energy of the system changed when the number of electrons in it is altered?

The first of these problems is connected with the study of the fermion branch of the spectrum (the problem of justifying the so-called "single-electron" theory, in particular, belongs to this group of problems), the second with the occurrence of boson-type excitations (excitons, plasmons, and so on), while the third one, in conjunction with the first one, covers the question of the influence of structural defects on the electron spectrum in solids. When talking about structural defects it is not necessarily required to have in view something inside the lattice: atoms (or molecules) adsorbed on the crystal surface can also play the role of "defects". In this way one can say that the problem of chemisorption falls within the framework of the electron theory of solids.

We must make two remarks in connexion with the statement of the problem which we just gave.

Firstly, it is clear that the semi-empirical approach (where we determine the electron spectrum in a perfect lattice from experimental data) can be successful only if one needs determine from the experimental data only a few parameters. (This is, for instance, the way in which effective mass problems are formulated; see Pekar 1951, Deĭgen and Pekar 1956, Slater 1949, Luttinger and Kohn 1955,

Kittel and Mitchell 1954.) It is from the beginning clear that one can only carry through such a programme for states which are described by sufficiently "smooth" wave functions (the long-wavelength part of the boson excitation spectrum, shallow localised states): only under those conditions can one take a "smeared out" periodic potential, the finer details of which do not play a role. On the other hand, for problems where wave numbers comparable with the reciprocal lattice constants are important, the semi-empirical approach may give results which are only of speculative interest. In particular, such an approach can hardly make sense, if we wish to evaluate the ground state energy of the many-electron system in a metal (unless we are interested in the purely methodological aspects of the problem).

Secondly, the first of the problems stated is of interest for semi-conductors, but not for metals. Indeed, the free electron concentration (and hence the average electron-electron interaction) can in semi-conductors, depending on the experimental conditions, vary between extremely large limits (without any change in the chemical nature of the substance). The problem of evaluating the energy spectrum parameters as functions of the free carrier concentration in the sample has thus a well-defined meaning. The idea of practically non-interacting conduction electrons has an equally well-defined meaning here, since their concentration may be made very small by a lowering of the temperature (the parameters of such a system are just those which are determined by diamagnetic resonance experiments in the microwave region). On the other hand, the electron concentration in a metal is practically always fixed, and the average electron-electron interaction energy is far from small compared with the average kinetic energy. The "free particle" spectrum concept has therefore lost here its physical meaning.

Recently a number of authors (Bohm and Pines 1952, 1953, Pines and Bohm 1952, Pines 1953, 1954, 1955, 1956a, b, Zubarev 1953, Kanazawa 1955, Adams 1955, Nozières and Pines 1958a, b, c, Bonch-Bruevich 1957b, c) have used "redundant variables" and obtained results connected with the study of the electronic energy spectrum in metals and semi-conductors (in particular, the study of the plasmon branch of the spectrum). The "redundant variable" method leads, however, in contradictinction to the Bose statistics case (Bogolyubov and Zubarev 1955) when applied to fermion systems to well-known, characteristic difficulties. First of all, the subsidiary conditions appearing in connexion with the introduction of redundant variables make the study of transport processes involving plasmons much more complicated. Secondly, the coupling between the fermion and the boson excitations which is assumed to be small by Zubarev (1953) and Bonch-Bruevich (1957b, c) is in actual fact apparently not small. Thirdly and finally, the artificial introduction of a limiting plasma momentum, k_c, is far from logically satis-

factory. The restriction upon the values of the wave vector should not be imposed, but should follow from the theory. In the following sections we shall see that when we solve the problem by Green function methods the theory itself, indeed, determines a "natural limit" for the plasma spectrum.

18. PLASMA OSCILLATION FREQUENCIES AND DAMPING

Let us consider a non-relativistic system of identically charged particles (in the following for the sake of simplicity simply called electrons) with purely electrostatic interactions and no magnetic field present. We shall assume that the system is neutral as a whole because of the presence of the (not necessarily uniformly spread out) classical compensating charge. Such a situation is typical both for metals (free electrons and the ions in the lattice) and for semi-conductors (free electrons or holes and charged impurity centres). If we consider the electrostatic interaction to occur through a field, we can immediately use (10.1), (10.2), (9.5a), and (9.13); we need only choose the particular form of the quantities $G_c^{(0)}$ and $D_c^{(0)}$ in accordance with the specific nature of the given physical system. We restrict ourselves to non-ferromagnetic substances. We shall also assume that the valence electrons are (energetically) sufficiently separated from all other electrons that we can consider the atomic cores simply as sources for the field *. It is natural to choose for the unperturbed problem, the solution of which is assumed to be known, the "single-electron" problem in a given perfect crystalline lattice. By "single-electron" we understand here the problem of one electron in the periodic field of the atomic cores which are neutralised by the uniformly distributed charge of all the other electrons. We assume that the corresponding energy eigenvalues are spin-independent ** and we denote them by $W(\lambda)$ and we denote the corresponding eigenfunctions by $\varphi_\lambda(\vec{x})$ (λ indicates here all quantum numbers except the spin-quantum number). The unperturbed fermion Green function is then according to (5.14) of the form

$$G_{c,ss'}^{(0)}(x,x') = -\frac{1}{2\pi}\Delta(s-s')\int d\lambda\ \varphi_\lambda(\vec{x})\ \varphi_\lambda^+(\vec{x}') \times \int_{-\infty}^{+\infty} d\omega\ e^{-i\omega(x_0-x_0')}\ \frac{\omega - W(\lambda) + i\varepsilon[2n^{(0)}(\lambda)-1]}{[\omega - W(\lambda)]^2 + \varepsilon^2}. \quad (18.1)$$

* Compare, however, the remark sub b at the beginning of section 22.

** We exclude thereby from our considerations not only ferromagnetics, but also substances for which spin-orbit coupling is important. We give in section 22 a generalisation to the case when the latter is, indeed, important.

Here $n^{(0)}(\lambda)$ is the occupation number in the state λ for the case where there are no interactions

$$n^{(0)}(\lambda) = \frac{1}{e^{-\beta\mu+\beta W(\lambda)} + 1} .$$

It is convenient for us in this chapter to separate off explicitly the chemical potential μ; the $W(\lambda)$ are then clearly the eigenvalues of the normal Hamiltonian rather than of the generalised Hamiltonian. We retain the notation E for the eigenvalues of the generalised Hamiltonian. We emphasise that we are talking now about a Hamiltonian which by definition does not contain particle-particle interactions. The spectrum $W(\lambda)$ is thus in general not the same as the experimentally determined one. In particular, the effective masses which will be introduced in the following will be "bare" masses (in the quantum field theory sense). These are in metals often different from the ones determined, for instance, from galvanomagnetic phenomena; in semi-conductors, on the other hand, one can encounter conditions when the electron-electron interaction practically vanishes, and the parameters characterising the function $W(\lambda)$ can then be determined directly from experimental data. The explicit evaluation of (18.1) is very difficult, as in actual fact the functions $\varphi_\lambda(\vec{x})$ can be effectively determined only in a very rough approximation. For this reason it is advisable, as we mentioned in the preceding section, to use one or other of the effective mass methods, considering the $\varphi_\lambda(\vec{x})$ as "effective" wave functions and to take the periodic field simply into account by introducing a few parameters in the unperturbed Hamiltonian. The system considered is then made spatially uniform (and we must therefore consider the compensating charge to be uniformly spread in space). It is well known that we must then distinguish two cases:

a. "Non-degenerate" case * (the case where there is only spin-degeneracy belongs to this class). The distances between the bands in the unperturbed problem are large compared with the characteristic interaction energies and we may neglect virtual interband transitions. We can then take the periodic field into account simply by replacing the kinetic energy operator by $W(-i\nabla_{\vec{x}})$ where $W(\vec{k})$ is the energy eigenvalue of the unperturbed problem and $\vec{k}$ the electron quasi-momentum (which strictly speaking varies within the first Brillouin zone).

b. "Degenerate" case. The distances between some of the bands is not very large, and we need take into account the corresponding virtual transitions. If we wish to take the periodic field into account we must here replace the usual kinetic energy operator by the second-rank matrix $T_{ij}(-i\nabla_{\vec{x}})$ where i and j run through a finite set of values;

* One should not confuse the "degenerate" and "non-degenerate" cases considered here with Fermi-degeneracy. As far as the statistics obeyed by the particles in the system are concerned, they may be either degenerate or non-degenerate in both case a and case b.

the "effective wave function" is then also a matrix. It is necessary to state the problem in this way, if the valence electrons are not too strongly separated energetically from all other electrons so that we must consider the electrons from the outer shells on the same footing as the valence electrons. We must also consider this case when there are several kinds of charged particles.

In the present section we shall only consider case a. In that case we get from (18.1)

$$G^{(0)}_{c,ss'}(x, x') = \Delta(s-s') \int d^4k \, e^{-i(\vec{k}\cdot\vec{x}-\vec{x}')} \, G^{(0)}_c(k) \, , \qquad (18.2)$$

where

$$G^{(0)}_c(k) = -\frac{1}{(2\pi)^4} \cdot \frac{k_0 - W(\vec{k}) + i\varepsilon\,[2n^{(0)}(\vec{k}) - 1]}{[k_0 - W(\vec{k})]^2 + \varepsilon^2} \, . \qquad (18.3)$$

The approximation used here is clearly somewhat less restrictive than the effective mass method in its standard form: we obtain the latter if we further approximate $W(\vec{k})$ by a quadratic expression in $\vec{k}$, but this is by no means always possible in metals. In that sense the usual terminology "effective mass method" is apparently not very felicitous (it would be better to talk of the "effective kinetic energy").

We can in the case considered assume that the vector potential of the electromagnetic field, which transfers the interaction between the particles, vanishes. There remains thus only the component $D_{c,00}$ of all the components of the $D_{c,\mu\lambda}(x, x')$ tensor:

$$D^{(0)}_{c,00}(x, x') = \int d^3\vec{k} \, d\omega \, e^{-i\omega(x_0-x'_0)+i(\vec{k}\cdot\vec{x}-\vec{x}')} \, D^{(0)}_{c,00}(\vec{k}, \omega) \, , \qquad (18.4)$$

where we can use the non-relativistic expression (5.39) for $D^{(0)}_{c,00}(\vec{k},\omega)$:

$$D^{(0)}_{c,00}(\vec{k}, \omega) \equiv D^{(0)}_c(\vec{k}, \omega) = \frac{1}{(2\pi)^4 \, \vec{k}^2} \, . \qquad (18.5)$$

This means, in particular, that the Maxwell equations in this case reduce to the Poisson equation. We draw attention to the fact that in the method developed here we have no difficulty with satisfying the Lorentz condition for the four-potential: it is automatically satisfied because of the special form, (5.35) and (9.15), of the tensors $D_{\mu\lambda}$ and $\mathcal{P}_{\mu\lambda}$; in the present case the Lorentz condition must, of course, be satisfied up to the terms of order $1/c^2$.

We note, finally, that in the present approximation $\Gamma^{(0)} = 1$.

It is clear from (18.5) (and was apparent from the beginning from the way the problem was stated) that in the present approximation there will be no boson-type excitations; in other words, $D^{(0)}_c(\vec{k},\omega)$ has no poles in the ω-plane (it does not depend at all on ω). It is, however, clear from (11.2) that in actual fact such excitations may occur, being caused by the particle-particle interaction (and with the redis-

tribution of the charge density connected with it *. For a study of this problem it is sufficient to find the complete boson Green function $D_C(\vec{k}, \omega)$, that is, the polarisation operator $\mathcal{P}(\vec{k}, \omega)$ of the system (see (11.2); because of the non-relativistic character of the problem the tensors $D_{\mu\lambda}(\vec{k}, \omega)$ and $\mathcal{P}_{\mu\lambda}(\vec{k}, \omega)$ reduce to scalars just as (5.35) was changed to (5.40)). Once we have evaluated the polarisation operator, and thus also $D_C(\vec{k}, \omega)$, we determine in accordance with the general theory of sections 4 and 5 the plasma oscillation spectrum by looking for the singularities of the spectral function

$$J(\vec{k}, \omega) = \frac{2 \operatorname{Im} D_C(\vec{k}, \omega)}{1 + e^{-\beta E}} .$$

From (11.2) and (18.5) we get

$$\operatorname{Im} D_C(\vec{k}, \omega) = \operatorname{Im} \frac{D_C^{(0)}(\vec{k})}{1 - (2\pi)^8 D_C^{(0)}(\vec{k})\, \mathcal{P}(\vec{k}, \omega)}$$

$$= \frac{(2\pi)^8 [D_C^{(0)}(\vec{k})]^2 \operatorname{Im} \mathcal{P}(\vec{k}, \omega)}{[1 - (2\pi)^8 D_C^{(0)}(\vec{k}) \operatorname{Re} \mathcal{P}(\vec{k}, \omega)]^2 + [(2\pi)^8 D_C^{(0)}(\vec{k}) \operatorname{Im} \mathcal{P}(\vec{k}, \omega)]^2} ,$$

and the problem reduces thus to finding the solution of the following equation **

$$[1 - (2\pi)^8 D_C^{(0)}(\vec{k}) \operatorname{Re} \mathcal{P}(\vec{k}, \omega)]^2 + [(2\pi)^8 D_C^{(0)}(\vec{k}) \operatorname{Im} \mathcal{P}(\vec{k}, \omega)]^2 = 0 , \quad (18.6)$$

or

$$1 - (2\pi)^8 D_C^{(0)}(\vec{k}) \operatorname{Re} \mathcal{P}(\vec{k}, \omega) \pm i (2\pi)^8 D_C^{(0)}(\vec{k}) \operatorname{Im} \mathcal{P}(\vec{k}, \omega) = 0 . \quad (18.6a)$$

Let the solution of this equation, which in general is a transcendental one, be $\omega(\vec{k}) = \omega_{pl}(\vec{k}) - i\gamma(\vec{k})$. Here, $\omega_{pl}(\vec{k})$ and $\gamma(\vec{k})$ are real functions and we must assume that $\gamma(\vec{k}) \geq 0$ (see chapter I). This determines the choice of sign in (18.6a). We have already noted several times (for instance, in section 16) that the concept of elementary excitations has a meaning only insofar as the damping is sufficiently small. In this connexion we assume from the start that $\omega_{pl} \gg \gamma$. We ascribe therefore formally a small parameter ϵ to the imaginary part of the polarisation operator and we shall try to find the solution of (18.6) or (18.6a) in the form of a power series in ϵ. In zeroth approximation $\omega_{pl}(\vec{k})$ is defined as the real root of the equation

$$1 - (2\pi)^8 D_C^{(0)}(\vec{k}) \operatorname{Re} \mathcal{P}(\vec{k}, \omega) = 0 . \quad (18.7)$$

* We must, of course, evaluate the polarisation operator $\mathcal{P}$ as a function of the complex argument ω when solving (18.6). We emphasise that this does not mean at all an analytical continuation of $D_C(k, \omega)$ into the complex plane: we know that this is impossible.

** One often studies the excitations which are oscillations of the volume charge density in connexion with gaseous discharge plasma physics. We shall call them plasma oscillations in accordance with our general terminology.

This is called a dispersion relation as it determines the quasi-particle dispersion law, that is, the form of the function $\omega_{pl}(\vec{k})$. We find further for the "damping constant" $\gamma(\vec{k})$

$$\gamma(\vec{k}) = \left| \frac{\text{Im } \mathcal{P}(\vec{k}, \omega_{pl}(\vec{k}))}{\frac{\partial}{\partial\omega} \text{Re } \mathcal{P}(\vec{k}, \omega)\Big|_{\omega=\omega_{pl}(\vec{k})}} \right| . \tag{18.8}$$

We must, of course, when solving for ω_{pl} and γ check that the inequality $\omega_{pl} \gg \gamma$ is satisfied. There are in this connexion three possibilities. Firstly, it may turn out that there is a range of wave vector values for which Im $\mathcal{P}(\vec{k}, \omega) = 0$, and thus $\gamma(\vec{k}) = 0$. Relation (18.7) will then be exact and its real roots define undamped oscillations. The complex roots of (18.7) are apparently of no interest as their real and imaginary parts will in general be of the same order of magnitude. Secondly, there is the possibility that Im $\mathcal{P}(\vec{k}, \omega_{pl}(\vec{k})) = 0$, where $\omega_{pl}(\vec{k})$ is a real root of (18.7). In the present approximation we have then $\gamma(\vec{k}) = 0$; in other words, the damping is of higher order in ε. Finally, it is possible - and we shall see in section 20 that this case actually occurs - that for well-defined values of $\vec{k}$ the inequality $\omega_{pl} \gg \gamma$ is not satisfied. This indicates that there can be no plasma oscillations with such wave numbers, providing us in this way with one of the "natural limits" to the plasma spectrum.

We note that it is far from trivial that there exist purely real roots of (18.7) (this might well not have been the case). We shall see in sections 19 and 20 that (18.7) possesses real roots only if k is sufficiently small; we obtain in that way another of the "natural limits" of the plasma spectrum. This fact was apparently first observed by Bonch-Bruevich (1957a). Sawada, Brueckner, Fukuda, and Brout (1957) and Brout (1957) obtained by a different method the same result a little later.

To evaluate the polarisation operator we shall use the improved perturbation theory of section 11. In the first non-vanishing approximation we get from (11.4)

$$\mathcal{P}(\vec{k}, \omega) = -\frac{2ie^2}{(2\pi)^8} \int d^3\vec{k}' \int_{-\infty}^{+\infty} d\omega' \, \frac{\omega' - W(\vec{k}') + i\varepsilon\,[2n^{(0)}(\vec{k}') - 1]}{[\omega' - W(\vec{k}')]^2 + \varepsilon^2}$$

$$\times \frac{\omega' - \omega - W(\vec{k}' - \vec{k}) + i\varepsilon\,[2n^{(0)}(\vec{k}' - \vec{k}) - 1]}{[\omega' - \omega - W(\vec{k}' - \vec{k})]^2 + \varepsilon^2} . \tag{18.9}$$

The factor 2 arises from the trace over the spin variable. We integrate over ω', closing the contour in the upper ω'-half-plane (in accordance with the rule (5.5)). We get

$$\mathcal{P}(\vec{k},\omega) = \frac{2e^2}{(2\pi)^7}\int d^3\vec{k}'\, n^{(0)}(\vec{k}')\left\{\frac{1}{W(\vec{k}') - W(\vec{k}'-\vec{k}) - \omega + i\varepsilon}\right.$$

$$\left. + \frac{1}{W(\vec{k}') - W(\vec{k}'+\vec{k}) + \omega + i\varepsilon} + \frac{2\, i\varepsilon\, n^{(0)}(\vec{k}'-\vec{k})}{[W(\vec{k}') - W(\vec{k}'-\vec{k}) - \omega]^2 + \varepsilon^2}\right\}. \tag{18.10}$$

We now bear in mind the well-known relations

$$\lim_{\varepsilon\to 0} \frac{\varepsilon}{x^2+\varepsilon^2} = \pi\,\delta(x)\ , \tag{18.11}$$

$$\lim_{\varepsilon\to 0} \frac{x}{x+\varepsilon^2} = \frac{1}{x}\qquad , \tag{18.12}$$

$$\lim_{\varepsilon\to 0} \frac{1}{x \pm i\varepsilon} = \frac{1}{x} \mp \pi\, i\, \delta(x)\ . \tag{18.13}$$

In these equations x is a real quantity and $1/x$ on the right-hand sides of (18.12) and (18.13) must be understood to imply taking the principal value of the expressions in which it occurs. We get now from (18.10), for real ω

$$\mathrm{Re}\ \mathcal{P}(\vec{k},\omega) = \frac{2e^2}{(2\pi)^7}\int d^3\vec{k}'\, n^{(0)}(\vec{k}')\, \mathcal{P}\left\{\frac{1}{W(\vec{k}') - W(\vec{k}'-\vec{k}) - \omega}\right.$$

$$\left. + \frac{1}{W(\vec{k}') - W(\vec{k}'+\vec{k}) + \omega}\right\} \tag{18.14}$$

The imaginary part of $\mathcal{P}$ occurs if for $\varepsilon = 0$ one of the denominators in (18.10) vanishes, that is, if for some value of k the following equation holds:

$$W(\vec{k}') - W(\vec{k}'\pm\vec{k}) \pm \omega = 0\ .$$

When we evaluate the damping using (18.8) we must substitute for ω everywhere the (real) plasma oscillation frequency $\omega_{pl}(\vec{k})$. The condition for the vanishing of the denominators is thus nothing but the energy (and momentum) conservation law which must be satisfied for real (but not for virtual) emission or absorption of plasmon quanta by the charge carriers. On the other hand, the corrections to the energy which are described by the real part (18.14) of the polarisation operator have no connexion whatever with this condition as they are caused by virtual processes. This fact is not at all peculiar for the specific case considered here, but is general in character.

For sufficiently long wavelengths (small k) the right-hand side of (18.14) can be approximately evaluated in the case which interests us at this moment without assuming a particular form for $W(\vec{k})$. We first

of all assume that the plasma frequency $\omega_{pl}(\vec{k})$ remains finite as $\vec{k} \to 0$; this will be justified by our subsequent calculations. We can then expand the right-hand side of (18.14) in a power series in k. We introduce the tensors

$$\mu_{ij} = \frac{3}{8\pi} \int d^3\vec{k}'\, n^{(0)}(\vec{k}') \frac{\partial^2 W(\vec{k}')}{\partial k_i' \partial k_j'}, \tag{18.15}$$

$$\sigma_{ijmn} = \frac{9}{8\pi} \int d^3\vec{k}'\, n^{(0)}(\vec{k}') \frac{\partial^2 W(\vec{k}')}{\partial k_i' \partial k_j'} \frac{\partial W(\vec{k}')}{\partial k_m'} \frac{\partial W(\vec{k}')}{\partial k_n'}, \tag{18.16}$$

$$\nu_{ijmn} = \frac{1}{32\pi} \int d^3\vec{k}'\, n^{(0)}(\vec{k}') \frac{\partial^4 W(\vec{k}')}{\partial k_i' \partial k_j' \partial k_m' \partial k_n'}. \tag{18.17}$$

As in (18.9) the integratuon over $\vec{k}'$ is here strictly speaking only over the first Brillouin zone. However, in some problems only a relatively small region of $\vec{k}'$-space is important (namely, the region where $n^{(0)}(\vec{k}')$ differs appreciably from zero). We can then without making serious errors integrate over the whole of $\vec{k}'$-space.

Using (18.15) to (18.17) we write (18.14), for finite ω, in the form

$$\mathrm{Re}\ \mathcal{P}(\vec{k}, \omega) = \frac{8e^2}{3(2\pi)^6} \cdot \frac{1}{\omega^2} \left\{ \mu_{ij} k_i k_j + \nu_{ijmn} k_i k_j k_m k_n + \sigma_{ijmn} \frac{k_i k_j k_m k_n}{\omega^2} \right\} + O(k^6). \tag{18.18}$$

It is clear that μ_{ij} is the average value (averaged over the region occupied by the electrons) of the inverse effective mass tensor; the tensors σ_{ijmn} and ν_{ijmn} characteristise finer details of the energy surface. Substituting (18.18) into (18.7) and using (18.5) we get in the approximation used here

$$\omega_{pl}^2(\vec{k}) = \frac{2e^2}{3\pi^2} \cdot \frac{k_i k_j}{k^2} (\mu_{ij} + \nu_{ijmn} k_m k_n) + \frac{\sigma_{ijmn} k_i k_j k_m k_n}{\mu_{ij} k_i k_j} + O(k^6)$$

This equation determines (for small values of k) the plasma frequencies in a solid for any degree of Fermi-degeneracy of the charge carriers and for any form of $W(\vec{k})$ (as long as the energy bands remain non-degenerate in the sense discussed earlier in this section). It is a generalisation of the results obtained by Wolff (1953) and makes these more precise; Wolff used an apparently insufficiently accurate method and thus did not find the term with ν_{ijmn} which characterises anisotropic systems. We could easily evaluate also the next terms of the expansions of Re $\mathcal{P}$ and ω_{pl} in powers of k, but they are of no interest as they are small. We note that (18.19) is not analytic as $k \to 0$ for the general case of arbitrary anisotropy: the

limiting frequency ω_0^2 depends on the orientation of $\vec{k}$. This result was obtained in a more general form and by another method by Pekar (1958).

One sees easily that the waves whose frequencies are given by (18.19) are longitudinal. Indeed, the electrical field strength is in this case simply given by the negative gradient of the scalar potential; it is thus for a given Fourier component parallel (or antiparallel) to $\vec{k}$. It follows from (18.19) that our assumption that $\omega_{\mathrm{pl}}^2(\vec{k})$ remains finite as $\vec{k} \to 0$ is valid only if the tensor μ_{ij} is non-vanishing. The equation $\mu_{ij} = 0$ holds, for instance, if a band is completely filled; we have then for all $\vec{k}'$, $n^{(0)}(\vec{k}') = 1$. If the tensor μ_{ij} vanishes, the expansion (18.18) is no longer tenable for $\omega = \omega_{\mathrm{pl}}$. One can, however, find a solution of (18.7) for small values of k also in this case; we get (for $\mu_{ij} = 0$, v, $\sigma \neq 0$)

$$\omega_{\mathrm{pl}}^2(\vec{k}) = a_{ij}\, k_i\, k_j\,, \tag{18.20}$$

where a_{ij} is a constant tensor. One can easily find the explicit form of a_{ij}.

We note that (18.19) has a meaning only if the quadratic form $\mu_{ij} k_i\, k_j$ is positive definite (ω_{pl} is real by definition). This condition does, however, not follow from some general physical considerations. It follows thus that a solution in the form (18.19) - which represents as we shall now see the ordinary plasma oscillations - is not possible for all forms of $W(\vec{k})$ and $n^{(0)}(\vec{k})$.

To elucidate definitely the physical nature of the excitations whose spectrum is given by (18.19) we shall evaluate the tensor μ_{ij} for the special case where $W(\vec{k})$ is a quadratic function

$$W(\vec{k}) = \tfrac{1}{2}\, m_{ij}^{-1}\, (k_i - k_i^{(0)})\, (k_j - k_j^{(0)})\,. \tag{18.21}$$

The $k_i^{(0)}$ are here the coordinates of the point where $W(\vec{k})$ is minimum, and the m_{ij}^{-1} are the components of the inverse effective mass tensor. The energy scale is chosen in such a way that $W(\vec{k}^{(0)}) \geq 0$. In particular, we have in the coordinate system in which the tensor m_{ij}^{-1} is on principal axes

$$W(\vec{k}) = \sum_{i=1}^{3} \frac{(k_i - k_i^{(0)})^2}{2m_i}\,. \tag{18.22}$$

We emphasise that even in a cubic crystal the principal values of the effective mass tensor m_1, m_2, and m_3 are not necessarily equal to one another. Indeed, the energy minimum may lie not at the centre of the Brillouin zone but at a point of lower symmetry * (so that $\vec{k}^{(0)}$ is different from zero). In that case $W(\vec{k})$ has then, of of course, not one, but several minima; their coordinates are interconnected through the symmetry transformations which are allowed

* This occurs, for instance, in germanium and silicon crystals (Dresselhaus, Kip, and Kittel 1955).

in the given crystallographic system. If the distances between the minima in $\vec{k}$-space are sufficiently large, one can write the integral in (18.15) - and also those in (18.16) and (18.17) - approximately as a sum of terms in each of which the integration is only over the vicinity of one of the minima. It is clear that when evaluating the integral it is sufficient to evaluate only one of the terms and then averaging over all orientations of $\vec{k}^{(0)}$ relative to the crystal axes. This is what we shall do in the following. We must, however, note that it is at the present time not clear in how far this approximation is justified for any particular crystal. We find in this way easily for a crystal with cubic symmetry

$$\mu_{ij} = \frac{3}{8\pi}\,\delta_{ij}\,\frac{1}{m^*}\int \mathrm{d}^3\vec{k}'\; n^{(0)}(\vec{k}')\;, \tag{18.23}$$

$$\frac{1}{m^*} = \frac{1}{3}\sum_{i=1}^{3}\frac{1}{m_i}\;. \tag{18.24}$$

The integral occurring in (18.23) is proportional to the total electron concentration

$$\frac{2}{(2\pi)^3}\int \mathrm{d}^3\vec{k}'\; n^{(0)}(\vec{k}') = n\;, \tag{18.25}$$

and we have thus

$$\mu_{ij} = \frac{3\pi^2}{2m^*}\,n\;\delta_{ij}\;. \tag{18.26}$$

One can also easily evaluate the tensors ν and σ. The first of these is in the present case clearly equal to zero and we find, after averaging, for the second

$$\sigma_{ijmn} = 3\;\pi^2\;\delta_{ij}\;\delta_{mn}\,n\,\frac{\widetilde{W}(T,n)}{m_i^2\;m_n}\;. \tag{18.27}$$

Substituting (18.26) and (18.27) into (18.19) and changing to the usual Gaussian system of units (which is done by changing e^2 to $4\pi e^2$) we get finally

$$\omega_{\mathrm{pl}}^2(\vec{k}) = \frac{4\pi n e^2}{m^*} + \frac{4}{\hbar^2}\,\widetilde{W}(T,n)\,\langle W(\vec{k})\rangle_{\mathrm{Av}} + O(k^4)\;. \tag{18.28}$$

Here $\widetilde{W}(T,n)$ is the average (unperturbed) electron energy and the symbol $\langle\ldots\rangle_{\mathrm{Av}}$ indicates an average over all minima. In particular, if $m_1 = m_2 = m_3 = m$ (isotropic model), $m^* = m$, and we get the well-known Langmuir formula for the limiting plasma frequency

$$\lim_{\vec{k}\to 0}\omega_{\mathrm{pl}}^2(\vec{k}) = \omega_0^2 = \frac{4\pi n e^2}{m}\;. \tag{18.29}$$

We remind ourselves that we must understand by e^2 the square of the

charge divided by the dielectric constant in a dielectric. The second term in (18.28) now takes on the well-known form

$$2\tilde{W}(T,n)\frac{\vec{k}^2}{m}\,. \tag{18.30}$$

It is clear from (18.23) that the value of the limiting frequency ω_0 is independent of the degree of degeneracy of the electron gas, as it is determined solely by the total particle concentration (the function $n^{(0)}(\vec{k})$ may be a fermion function or a boson function).

It is also clear that our method allows us, indeed, to obtain easily both the well-known classical expression for the plasma frequency and the generalisation of this expression for the case of an arbitrary anisotropy of the energy surfaces. This should not cause any astonishment as we have in fact followed closely the usual procedure to look for the plasma frequencies (see, for instance, the survey article by Gershman, Ginzburg, and Denisov (1957)). Indeed, the plasma frequencies are defined in the classical theory as the roots of the equation Re $\epsilon(\omega, \vec{k}) = 0$. We saw, however, in section 11 that the expression $1 - (2\pi)^8 D_C^{(0)} \mathcal{P}$ plays just the role of a generalised dielectric constant. Equation (18.7) is thus exactly the same as the equation Re $\epsilon(\omega, \vec{k}) = 0$ *. However, even in this case the Green function has some well-known advantages over the usual transport equation method, since

a. it gives an expression which is valid not only in the classical, but also in the quantum-mechanical region;
b. it allows us to establish easily the practical limits of the applicability of the equations obtained (see the next two sections and also section 11).

The subsequent study of the plasma spectrum, and in particular the study of the damping and of the natural limits of the spectrum can be most conveniently made separately for the completely degenerate and for the non-degenerate gas; we shall call these respectively the Fermi and the Boltzmann case.

19. ELECTRON GAS PLASMA SPECTRUM; FERMI CASE **

In this section we shall study the electron plasma in a metal for the case where we may assume the electron system to be completely degenerate: if there were no interactions, all states with energies lower than μ are occupied, while all states with energies above μ are free. We have thus

$$n^{(0)}(\vec{k}') = \theta\left[\mu - W(\vec{k}')\right], \tag{19.1}$$

* We note also that one could also obtain the formula for ω_0^2 directly from the expression (14.35) for the real part of the dielectric constant.

** Bonch-Bruevich (1957a), (1958a, b).

and we get for the average energy $\widetilde{W}$ using the quadratic approximation (18.22) $\widetilde{W} = \frac{3}{5}\mu$. We have thus

$$\omega_{\mathrm{pl}}^2(\vec{k}) = \frac{4\pi e^2}{m^*} + \frac{12\mu}{5\hbar^2} \langle W(\vec{k}) \rangle_{\mathrm{Av}} + O(k^4) \ . \tag{19.2}$$

The temperature does, of course, not enter into (19.2) as we used the condition of total degeneracy (19.1); the Green functions are then defined through an averaging over the ground state of the system.

In the isotropic case ($m_1 = m_2 = m_3 = m$) the second term on the right-hand side of (19.2) takes on the well-known form $(\frac{3}{5} v_{\mathrm{F}})^2 k^2$, where $v_{\mathrm{F}} = \sqrt{2\mu/m}$ is the velocity on the Fermi surface.

We note, however, that as far as applications to metals are concerned (19.2) has only methodological interest: in a real metal one can not, as a rule, reduce $W(\vec{k})$ to the simple quadratic form (18.22), and $W(\vec{k})$ is in general a much more complicated function of $\vec{k}$. We must therefore use for an evaluation of the plasma frequencies the general formulae (18.19) and (18.15) to (18.17) with (19.1) for $n^{(0)}(\vec{k}')$. For cubic crystals one can also use (14.35) and determine the plasma frequencies from the condition Re $\epsilon(\omega, \vec{k}) = 0$.

Let us now turn to the problem of the damping and of the limits of the plasma spectrum. Using (18.11) to (18.13) we find directly from (19.2) that for real ω and sufficiently small k the imaginary part of the polarisation operator (18.10) vanishes. Indeed, we saw that the occurrence of a finite imaginary part of $\mathcal{P}$ for real values of ω is connected with the vanishing of the denominators of (18.10):

$$W(\vec{k}') - W(\vec{k}' \pm \vec{k}) \pm \omega = 0 \ . \tag{19.3}$$

For small k we have

$$W(\vec{k}') - W(\vec{k}' \pm \vec{k}) \approx \mp k_i \frac{\partial W(\vec{k}')}{\partial k_i'} = \mp k_i v_i \ ,$$

where $\vec{v}(\vec{k}) = \nabla_{\vec{k}} W(\vec{k})$ is the velocity of an electron with quasi-wavevector $\vec{k}$. Moreover, we must substitute for ω the quantity $\omega_{\mathrm{pl}}(\vec{k})$ which is of interest to us. Condition (19.3) then becomes

$$|(\vec{k} \cdot \vec{v}(\vec{k}))| = \omega_{\mathrm{pl}}(\vec{k}) \ , \qquad W(\vec{k}) \leq \mu \ . \tag{19.4}$$

In other words, the imaginary part of the polarisation operator can under these conditions be different from zero only, if

$$v(\vec{k}) \geq \frac{\omega_{\mathrm{pl}}(\vec{k})}{k} \ , \qquad W(\vec{k}) \leq \mu \ , \tag{19.5}$$

that is, in particular,

$$v_{\max} \geq \frac{\omega_{\mathrm{pl}}(\vec{k})}{k} \ , \qquad W(\vec{k}) \leq \mu \ . \tag{19.6}$$

Here $v_{\max}$ is the maximum velocity of the electrons; if the velocity $v(\vec{k})$ increases monotonically with the energy, $W(\vec{k})$, we have

$v_{max} = v_F$. Equation (19.6) determines implicitly the lower limit of the wave vectors for which damping takes place.

Equation (18.6) has thus for sufficiently small values of k purely real solutions, that is, in the present approximation plasma waves of sufficiently long wavelengths will in a metal not be damped at all*. The reason for this is immediately clear from (19.5) and (19.6): when there are no interactions with the lattice vibrations, impurities, and so on, the plasma oscillation damping is caused only by the transfer of their energy into the fermion branch. For sufficiently long wavelengths this transfer is, however, impossible since the phase velocity of the plasma waves (the right-hand side of (19.5)) is larger than the maximum electron velocity.

The value of k determined by (19.6) might be taken to be the natural upper limit of the plasma spectrum. At longer wavelengths the plasma vibrations begin to be damped. We noted, however, already in section 18 that there may be also another reason for the occurrence of a natural limit to the plasma spectrum: (18.7) does not necessarily possess real roots for arbitrary k. To study this problem we must evaluate explicitly $\mathcal{P}(\vec{k}, \omega)$ for all values of its arguments which is clearly possible only if the form of $W(\vec{k})$ is known. In actual fact, however, $W(\vec{k})$ is known only for sufficiently small wave vectors (for values of k close to the inverse lattice constant the effective mass method itself becomes useless). It is therefore sensible to consider a model system, but the results obtained in that way will, in general, only be of methodological value. An exception is the case when the real solutions of (18.7) vanish already for rather small k. We shall see in the next section that this occurs, indeed, for a Boltzmann plasma in semiconductors. We shall restrict ourselves here to the simplest case - the quadratic isotropic approximation - and we put

$$W(\vec{k}) = \frac{\vec{k}^2}{2m}. \tag{19.7}$$

One can then easily completely evaluate the polarisation operator (18.10). It is convenient to introduce dimensionless variables, expressing k in units $k_F = mv_F$ and ω in units μ (we retain for the new

* We are considering here only the damping caused by the electron-electron interaction. In actual fact, the plasma waves in a solid are always damped because of the scattering of the electrons by lattice imperfections (phonons, atomic impurities, and so on). In a metal, however, this fact is unimportant since the corresponding "damping periods" (which are of the order of magnitude of the mean time of free flight) are large compared to the plasma oscillation periods. We note that we could easily study this damping within the framework of the method discussed here, if we wish to do so: we need only introduce in the Hamiltonian of the system the energy of the interaction of the electrons with the corresponding fields (for instance, phonons).

variables the old symbols, bearing in mind that this should not lead to misunderstandings). Integrating we get from (18.14)

$$\text{Re } \mathcal{P}(\vec{k},\omega) = \frac{g^2}{(2\pi)^4}\left\{\frac{4k^2 - \omega^2 - k^4}{8k^3}\ln\left|\frac{\omega^2 - (2k - k^2)^2}{\omega^2 - (2k + k^2)^2}\right|\right.$$

$$\left. - \frac{\omega}{4k}\ln\left|\frac{(\omega - 2k)^2 - k^4}{(\omega + 2k)^2 - k^4}\right| - 1\right\}, \qquad (19.8)$$

where

$$g^2 = \frac{2e^2}{\hbar v_F}. \qquad (19.9)$$

The charge e is here expressed in Gaussian units. The quantity g^2 plays the role of the dimensionless coupling constant and is in general not at all small.

If we expand the right-hand side of (19.8) for small k and finite ω, we get, of course, again (18.18), proviced we substitute there the appropriate values of the tensors μ, ν, and σ. On the other hand, it is immediately clear from (19.8) that for real ω and $k \sim 1$ (that is, for wavevectors of the order of the Fermi-wavevector) Re $\mathcal{P}(\vec{k},\omega) < 0$, and the dispersion relation (18.7) has therefore no real roots (the imaginary part of the polarisation operator may still be equal to zero). The natural limit to the plasma oscillation spectrum ($k \leq k_c$) is thus not imposed, but follows from the theory itself. The determination of the limiting wavenumber k_c reduces to a study of the region where real roots of (18.7) occur, when (19.8) is taken into account. We shall not do this, however, as the whole calculation is only of methodological interest, as we noted earlier.

We now go over to an estimate of the accuracy of the approximation used, using the renormalisation group according to the general scheme of section 11. It is sufficient to consider only the simplest case of the isotropic quadratic approximation (19.7) if we wish to elucidate the basic features of the problem.

We have done all necessary calculations already in section 11; we only need find an explicit expression for the function f occurring in (11.20). We put, as in section 11, $\hbar = 2m = 1$ and $W_0 = \mu$. We have then from (11.15) $u/v = \vec{k}^2/\mu \equiv z$, and we get from (11.13) and (19.8)

$$f(z) = \frac{1}{(2\pi)^2 z}\left\{\frac{4 - z}{4\sqrt{z}}\ln\left|\frac{2 - \sqrt{z}}{2 + \sqrt{z}}\right| - 1\right\} \leq 0. \qquad (19.10)$$

Equation (19.10) determines together with (11.19) and (11.22) the invariant charge which in actual fact will be our expansion parameter. As $f(z) < 0$ for any finite z, it is clear that the invariant - screened! - charge is in fact always less than g as was pointed out in section 11. In particular, in the small momentum region ($u \to 0$) the invariant charge tends to zero and our approximation for $d(u,v;g^2)$

becomes arbitrarily accurate *. This fact turns out to be important in connexion with the screening law for the external field (see section 22). On the other hand, in the "plasma" case in which we are interested here the invariant charge is given by

$$\frac{2\,e^2/\hbar v_F}{1 - 2\,\frac{e^2}{\hbar v_F} f\left(\frac{\omega_{pl} + \vec{k}^2}{\mu}\right)} < 2\,\frac{e^2}{\hbar v_F}\,, \tag{19.11}$$

as is clear from (11.22) and (11.30).

From this it is clear

a. that the actual expansion parameter depends on the wavevector and the frequency, and is not necessarily the dimensionless constant g^2; in other words, our problem of determining the plasma frequencies is justified in the sense that the subsequent terms in the expansion are not simply powers of g^2/ω^2;
b. that the practical degree of applicability of the expansion for small k is determined by the ratio of the plasma frequency and the Fermi energy so that the approximation is the better the larger the ratio μ/ω_{pl}.

This last fact is not connected with the approximation (19.7); however, specific numerical estimates of the expansion parameter depend, of course, on the form of the energy surfaces. A closer study shews that for the quadratic approximation (19.7) a sufficient condition for our expansion to be applicable in the plasma frequency region is the inequality

$$\frac{e^2/\hbar v_F}{1 + 2\sqrt{e^2/\pi\hbar v_F}} \ll 1\,. \tag{19.12}$$

For typical values of electron concentrations, n, in metals we get on the left-hand side of (19.12) a quantity close to unity. One should, however, bear in mind that in a metal the quadratic approximation hardly can be applied; the equations obtained using that approximation refer, strictly speaking, not to a metal, but to a model problem of a free electron gas. Inequality (19.12) it the condition for the applicability of the so-called high-density approximation. It is satisfied the better, the higher the electron concentration and the smaller their effective mass. In that sense we can consider the method discussed here as an improvement of simple expansions in the coupling constant (19.9) which have often been applied by different authors (see, for instance, Sawada, Brueckner, Fukuda, and Brout 1957, Brout 1957).

* One can easily verify that this statement is not connected with the assumption (19.7). It indicates merely the impossibility to propagate waves with zero energy and finite momentum (that is, it indicates the absence of real poles of the boson Green function for $\omega = 0$ and $k \neq 0$).

20. ELECTRON GAS PLASMA SPECTRUM; BOLTZMANN CASE *

The plasma spectrum of a Boltzmann electron gas has often been studied in connexion with gas discharge physics problems. A number of the results obtained then can immediately be transferred to the semi-conductor case, by a simple change in notation. Semi-conductors have, however, also well-known specific peculiarities and this makes the study of electron (or hole) plasmas of interest beyond a purely methodological one. The free electron concentration in semi-conductors is, as a rule, larger (sometimes considerably larger) than those in a gas discharge; plasma effects in semi-conductors are thus far more pronounced. We must also bear in mind that one can relatively easily vary the free charge concentration in a semi-conductor experimentally within wide limits, while all other conditions remain unchanged. When the electron concentration is increased in comparison with that in a gas discharge we get to another peculiarity of the plasma in semi-conductors: there may occur here rather appreciable quantum effects. Indeed, the latter comes into play as soon as the average distance between the electrons ($\sim n^{-1/3}$) becomes comparable with the "thermal" wavelength $\lambda_T = h\sqrt{\beta/m}$. Finally, in contradistinction to a gas discharge, one can when studying plasma phenomena in semi-conductors practically always assume that the heavy particles (donors, acceptors, ...) remain stationary; we need thus deal with a bipolar plasma only in the case of intrinsic conduction. For semi-conductors such as germanium and silicon most interest attaches just to a study of a plasma with one kind of free charges since in such samples one can most easily reach the required large charge carrier concentrations.

When applying the methods of section 18 to semi-conductors we must bear in mind the following facts.

Firstly, in semi-conductors the total concentration of electrons - which we have all the time assumed to be given - is, strictly speaking, not given, but can fluctuate (as the charge carriers are created by heat motion). In actual fact, however, this does not change the calculations as the recombination time (which determines the rate of change of n) is, as a rule, several orders of magnitude larger than the plasma oscillation period.

Secondly, since the recombination process is a slow one the charge carrier concentration may even be a non-equilibrium one: non-equilibrium electrons and holes, injected into the sample by light or by an electrical field, can also take part in plasma effects, until they recombine.

Thirdly, we shall see that all plasma effects in semi-doncuctors occur in the region of relatively small wavenumbers, when the approximation (18.22) is rather reliable. We remind ourselves that we

* Bonch-Bruevich and Kogan 1959, Bonch-Bruevich and Mironov 1960.

are considering the case of non-degenerate bands (in the sense of section 17). We shall consider the degenerate case in section 22. The results which we shall obtain will thus be of more than just methodological value. We shall in the present section use everywhere the approximation (18.22).

Fourthly, in contradistinction to the case of metals, the plasma oscillation periods in semi-conductors are usually (for typical electron concentrations) comparable to the mean free flight times (caused by scattering by phonons, impurities, and so on) or, at any rate, not much larger. The plasma frequencies which we obtained from (18.7) will thus in actual fact be only the "centres of gravity" of rather wide lines, and one can not consider damping adequately without taking into account of the interaction of the charge carriers with phonons, impurities, and so on.

If there is no interaction, the distribution function will in the present case be given by

$$n^{(0)}(\vec{k}) = e^{\beta\mu - \beta W(\vec{k})} , \tag{20.1}$$

where we must assume in accordance with our present approximation that $n^{(0)}(\vec{k}) \ll 1$, and retain everywhere only quantities of first order in $n^{(0)}(\vec{k})$. We have thus

$$\widetilde{W} = \frac{3}{2\beta} \equiv \frac{3}{2} k_B T ,$$

and (18.27) becomes

$$\omega_{pl}^2 = \frac{4\pi n e^2}{m^*} + \frac{3 k_B T \vec{k}^2}{m^*} + O(k^4) . \tag{20.2}$$

We get from this, in particular, in the isotropic approximation the well-known result

$$\omega_{pl}^2 = \frac{4\pi n e^2}{m} + \frac{3 k_B T}{m} \vec{k}^2 . \tag{20.3}$$

On the other hand, for sufficiently large values of k, (18.7) has, as in the fermion gas case, no real roots. One verifies this easily by evaluating the real part of the polarisation operator for real values of ω. In the approximation (18.22) we get (in Gaussian units)

$$\mathrm{Re}\, \mathcal{P}(\vec{k}, \omega) = - \frac{4ne^2}{(2\pi)^3 \hbar} \sqrt{\frac{\beta}{W(\vec{k})}} \int_0^\infty dx\, e^{-x^2} \cos\left(\frac{\beta\omega x}{\sqrt{\beta W(\vec{k})}}\right) \sin\left(x \sqrt{\beta W(\vec{k})}\right) . \tag{20.4}$$

One can easily express the right-hand side in terms of a Fresnel integral, but it is more convenient to leave it in the present form. Expanding the integral in a power series in $\vec{k} - \vec{k}^{(0)}$ (for finite ω) and afterwards averaging over all possible orientations of $\vec{k}^{(0)}$ leads again to (20.2). On the other hand, if $|\vec{k} - \vec{k}^{(0)}|$ is sufficiently large, one sees easily that the right-hand side of (20.4) becomes negative:

a study of (18.7) with the real part of the polarisation operator in the form (20.4) (and $\vec{k}^{(0)} = 0$) shews that there are real roots, only if

$$k < k_c \cong \frac{0.53}{r_D}, \tag{20.5}$$

where

$$r_D = (4\pi n e^2 \beta)^{-\frac{1}{2}} \tag{20.6}$$

is the Debye radius (in Gaussian units). We see thus that also in the Boltzmann case the existence of a natural limit to the plasma spectrum is not imposed ad hoc, but follows from the theory itself (see, however, the discussion following (20.13)).

If we now turn to the damping caused by the Coulomb interaction between the electrons, we note first of all that now, in contradistinction to the Fermi case, the imaginary part of the polarisation operator never vanishes exactly. Indeed, in a Boltzmann gas are particles moving with any velocity we choose; inequality (19.5) can thus be satisfied for any k (that is, there are always electrons with velocities which exceed the phase velocity of the plasma wave *). It follows from this that (18.6) can not possess purely real solutions, and that the plasma waves are always damped, whatever the value of k. When we evaluate the imaginary part of the polarisation operator $\mathcal{P}(\vec{k}, \omega)$ we must thus at once put (compare section 5)

$$\omega = \omega' - i\omega'', \quad \omega'' > 0. \tag{20.7}$$

We can then at once neglect ϵ in (18.10), since $W(\vec{k})$ is real so that the denominators have no zeroes.

We get then from (18.10)

$$\operatorname{Im} \mathcal{P}(\vec{k}, \omega) = \frac{2e^2}{(2\pi)^7} \operatorname{Im} \int d^3\vec{k}'\, n^{(0)}(\vec{k}') \left\{ \frac{1}{W(\vec{k}') - W(\vec{k}'-\vec{k}) - \omega' + i\omega''} + \frac{1}{W(\vec{k}') - W(\vec{k}'+\vec{k}) + \omega' - i\omega''} \right\}. \tag{20.8}$$

The evaluation of the integral on the right-hand side in its general form is somewhat cumbersome. This is, however, unnecessary, as we are in the following interested only in the value of the polarisation operator for $\omega' = \omega_{pl}$, $\omega'' = \gamma$; we may thus assume that $\omega' \gg \omega''$. We can then use (18.13) considering ω'' formally to be an infinitesimally small quantity,

* We bear in mind that we are dealing here with a non-relativistic theory and that there is thus no limit to the electron velocity. It is true that if k is sufficiently small the velocities which satisfy (19.5) may become so large that one can no longer apply the non-relativistic approximation. It will be clear from the following, however, that under those conditions the damping connected with the Coulomb interaction between the electrons is far from small and this mechanism is unimportant compared to other causes leading to the dissipation of the plasma wave energy.

$$\frac{1}{W(\vec{k}') - W(\vec{k}'\pm\vec{k}) \pm \omega' \mp i\omega''} \cong \frac{1}{W(\vec{k}') - W(\vec{k}'\pm\vec{k}) \pm \omega'} \pm \pi i \delta \left[W(\vec{k}') - W(\vec{k}'\pm\vec{k}) \pm \omega'\right] . \quad (20.9)$$

From (20.9) we get

$$\text{Im } \mathcal{P}(\vec{k}, \omega') = -\frac{2e^2}{(2\pi)^6} \int d^3\vec{k}' \, n^{(0)}(\vec{k}') \{\delta \left[W(\vec{k}') - W(\vec{k}'-\vec{k}) - \omega'\right) - \delta \left[W(\vec{k}') - W(\vec{k}'+\vec{k}) + \omega'\right]\} . \quad (20.10)$$

This is the limiting value of Im $\mathcal{P}(\vec{k}, \omega)$ as $\omega'' \to 0$, that is, is is the expression we need to evaluate γ from (18.8). In the approximation (18.22) when $W(\vec{k})$ is a quadratic expression, one can easily evaluate the integral occurring here for any degree of degeneracy of the electron gas. In the Boltzmann case, in particular, when $n^{(0)}(\vec{k})$ is given by (20.1) we get (using here Gaussian units)

$$\text{Im } \mathcal{P}(\vec{k}, \omega') = \frac{ne^2 \sqrt{2\beta} \exp\left(-\frac{\beta W(\vec{k})}{4} - \frac{\beta\omega'^2}{4W(\vec{k})}\right)}{(2\pi)^{5/2} \hbar \sqrt{W(\vec{k})}} \sinh \tfrac{1}{2} \beta \hbar \omega' . \quad (20.11)$$

Since we know already the real part of the polarisation operator we can easily find from (18.8) the damping of the plasma oscillations. For small wavevectors, in particular, we get (in Gaussian units)

$$\gamma = \sqrt{\frac{\pi}{2}} \frac{\sinh \frac{1}{2} \beta \hbar \omega_{pl}}{(kr_D)^3 \beta \hbar} \exp\left(-\frac{1}{2(kr_D)^2}\right) . \quad (20.12)$$

This expression reduces to Landau's well-known expression (1946) as $\hbar \to 0$.

Because the damping is finite, the question of the natural limit of the plasma spectrum becomes, as always in such cases, somewhat arbitrary. The presence of many scattering mechanisms leads also to additional complications. We shall therefore not consider it in detail; we note merely that both (20.5) and the condition that γ be sufficiently small compared with ω_{pl} give about the same value for the critical wave number k_c. Indeed, if we substitute the value $k = k_c/2$ into (20.12), we get * $\gamma \cong 0.05\, \omega_{pl}$: the damping is still small; on the other hand, for $k = k_c$ we get $\gamma \cong \omega_{pl}$ from (20.12).

In semi-conductors the Debye radius is, as a rule, at least two or three orders of magnitude larger than the lattice constant. The plasma wavelengths turn thus out to be, indeed, very large and this justifies the use of (18.22). We note also that under the conditions

* We must bear here in mind that under conditions which are typical for semi-conductors (and at room temperature) $\sinh \frac{1}{2} \beta \hbar \omega_{pl}$ is less than unity.

mentioned all plasma frequencies lie in a very narrow region which differs from ω_0 only by 10 to 15 per cent.

We shall now estimate the accuracy of the approximation used, employing the renormalisation group. As in sections 11 and 19 we restrict ourselves to the isotropic approximation, and put

$$W(\vec{k}) = \frac{\vec{k}^2}{2m} . \tag{20.13}$$

In contradistinction to section 19, we have now not one independent dimensionless parameter, containing the charge e, but several. We are therefore unable to fix a priori the form of the dimensionless constant g, but we must determine it from the condition that we can write the product $(2\pi)^8 \mathcal{P}^{(0)}(\vec{k}, \omega) D^{(0)}(\vec{k})$ in the form (11.20). Using (5.39) and (20.4) we see easily that in the present case the quantity $\beta^{-1} = k_B T$ plays the role of the parameter W_0; we get for f:

$$f(\frac{u}{v}) = - (\frac{v}{u})^{\frac{3}{2}} \int_0^\infty dt\ e^{-t^2} \sin (t \sqrt{\frac{u}{v}}) \equiv - (\frac{v}{u})^{\frac{3}{2}} S(\frac{u}{v}) , \tag{20.14}$$

where

$$S(z) = e^{-z} \int_0^{\sqrt{z}/2} e^{t^2} dt .$$

Moreover,

$$g^2 = 2 \frac{W(\vec{k})}{k_B T}\bigg|_{k=r_D^{-1}} = (\frac{\hbar \omega_0}{k_B T})^2 . \tag{20.15}$$

Introducing an effective number of states in the band by

$$N_{st} = \frac{2(2\pi m k_B T)^{\frac{3}{2}}}{(2\pi\hbar)^3} \tag{20.16}$$

and the "thermal velocity",

$$v_T = \sqrt{\frac{3 k_B T}{m}} , \tag{20.17}$$

we can write the coupling constant (20.15) in the form (in Gaussian units)

$$g^2 = 4 \sqrt{\frac{3}{2\pi}} \cdot \frac{e^2}{\hbar v_T} \cdot \frac{n}{N_{st}} . \tag{20.18}$$

This quantity is not necessarily very small; we saw, however, in section 11 that it is not the expansion parameter. The role of the latter is for the determination of $D_c(\vec{k}, \omega)$ at $\omega = 0$ played by the invariant charge (11.22)

$$g^2_{inv}(u, v; g^2) = \frac{g^2}{1 - g^2 f(\frac{u}{v})} .$$

In the present case we have from (20.14)

$$g^2_{\text{inv}}(u, v; g^2) = \frac{g^2}{1 + g^2 \left(\frac{v}{u}\right)^{\frac{3}{2}} S\left(\frac{u}{v}\right)}. \tag{20.19}$$

As we should have expected, $g^2_{\text{inv}} < g^2$ for all values of u and v. In particular, for small wave numbers ($k \ll r_D^{-1}$) one can get the expansion parameter g^2_{inv} as small as one wants.

Moreover, it appears from (11.30) that when we determine $D(\vec{k}, \omega)$ for non-vanishing values of ω (that is, in particular, when determining the plasma frequencies ω_{pl}) we get for the expansion parameter the quantity

$$g^2_{\text{inv}}(t, v; g^2) = \frac{g^2}{1 + g^2 \left[\frac{k_B T}{\hbar\omega + W(\vec{k})}\right]^{\frac{3}{2}} S\left[\frac{\hbar\omega + W(\vec{k})}{k_B T}\right]}. \tag{20.20}$$

From this follows, as in section 19, that our method of determining the plasma frequencies is always correct in the sense that the next terms in the expansion are not of the form of a power of g^2/ω^2. The condition that one can in fact apply the expansions used here is determined by the ratio of $k_B T$ to the plasma frequency: the convergence is the better the larger the ratio $k_B T/\omega_{pl}$.

21. SCREENING OF A STATIC FIELD BY FREE CHARGES *

When studying the fermion branch of the energy spectrum using, for instance, (9.18) we need know $\tilde{\varphi}$, the average (screened) potential created by the classical field sources (for instance, charged donors and acceptors in semi-conductors). We saw in section 8 that in the linear approximation

$$\tilde{A}_\beta(x) = - \int d^4y \, D'_{c,\beta\gamma}(x, y) \, J^\gamma(y) \, .$$

Here, $D'_{c,\beta\gamma}$ is the Green function evaluated for the case where there is no field. If we now substitute for D'_c the "unperturbed" value $D'^{(0)}_c$ of (18.5) we get an expression for the potential $\tilde{A}_\beta$ in a space which does not contain any free charges. Replacing $D'^{(0)}_c$ by D'_c means taking into account the reaction of the free charges on the external field, that is, taking screening into account.

At the moment we are interested only in the component $\tilde{A}_0 = - \tilde{\varphi}$; the classical current density J^γ is reduced to the charge density $J^0 = \rho(\vec{x})$. We write D'_c and ρ in Fourier series; we then get from (11.6) to (11.8)

* Bonch-Bruevich (1958a, b); Bonch-Bruevich and Kogan 1959.

$$\tilde{\varphi}(\vec{x}) = \int d^3\vec{k}\, \frac{e^{i(\vec{k}.\vec{x})}}{\vec{k}^2} \frac{\rho(\vec{k})}{1 - \frac{(2\pi)^4}{\vec{k}^2} \mathcal{P}(\vec{k}, \omega)\Big|_{\omega=0}} . \tag{21.1}$$

We note that $\mathrm{Im}\, \mathcal{P}(\vec{k}, 0) = 0$, $\mathrm{Re}\, \mathcal{P}(\vec{k}, 0) < 0$, as should be the case.

We shall especially consider the case of a point charge, when

$$\rho(\vec{y}) = e\, Z\, \delta(\vec{y}) , \tag{21.2}$$

where Z is an integer. The problem of the screening of the field of such a centre by free particles has often been considered. The screening law turns out to be an exponential one in the Debye approximation (we use in (21.3) to (21.9) Gaussian units):

$$\tilde{\varphi}(\vec{x}) = \frac{Ze}{r} e^{-r/r_D} , \qquad r \equiv |\vec{x}| . \tag{21.3}$$

On the other hand, the cut-off of the long-wavelength components of the field in the redundant variable method (see Pines 1956a, Bonch-Bruevich 1957b, c) gives

$$\tilde{\varphi}(\vec{x}) = \frac{Ze}{r} \cdot \frac{2}{\pi} \int_{k_c r}^{\infty} \frac{\sin u}{u}\, du , \tag{21.4}$$

where k_c is the "limiting" plasma wave number.

We shall shew that in actual fact these two laws are not in contradiction to one another, but are two different asymptotic forms of a more complicated expression.

To begin with we consider the simplest case where $W(\vec{k}) = \vec{k}^2/2m$. We can then integrate on the right-hand side of (21.1) over the polar angles of $\vec{k}$ (we choose the vector $\vec{x}$ as our polar axis). This leads to

$$\tilde{\varphi}(r) = \frac{Ze}{r} \cdot \frac{1}{(2\pi)^2} \int_0^{\infty} dk\, \frac{\sin kr}{k} \cdot \frac{1}{1 - \frac{(2\pi)^4}{k^2} \mathcal{P}(k, 0)} . \tag{21.5}$$

Small values of k are the most important ones in the integral for large distances from the origin. We can thus approximately replace $\mathcal{P}(k, 0)$ by its value for $k = 0$, and we get from (21.5)

$$\tilde{\varphi}(r) = \frac{Ze}{r} e^{-r/r_0} , \tag{21.6}$$

where

$$r_0^{-1} = (2\pi)^2 \sqrt{|\mathcal{P}(0,0)|} . \tag{21.7}$$

We note that if we want to evaluate $\mathcal{P}(0, 0)$, for instance, by using (18.10), we need, of course, be careful. In the case considered here, however, we can use the explicit expressions (19.8) and (20.4). This leads to

(Fermi case) $$r_0^{-1} = \sqrt{\frac{4}{\pi}}\sqrt{\frac{e^2}{\hbar v_F}}k_F = 2\left(\frac{3}{\pi}\right)^{\frac{1}{6}}\sqrt{\frac{me^2}{\hbar^2}n^{\frac{1}{3}}}, \qquad (21.8)$$

where k_F is the value of the wavenumber on the Fermi surface; or

(Boltzmann case) $$r_0^{-1} = \sqrt{4\pi\beta ne^2} = r_D^{-1}. \qquad (21.9)$$

We see thus that (21.6) is the usual Debye law. The distances for which we have obtained it here are determined by the condition

$$n(k) \cong 0 \quad \text{if} \quad k \gtrsim r_0^{-1}. \qquad (21.10)$$

In the Fermi case (21.10) becomes

$$r \gg r_c \equiv k_F^{-1} = (3\pi^2 n)^{-\frac{1}{3}}, \qquad (21.10a)$$

and in the Boltzmann case

$$r \gg r_c \equiv \frac{\hbar\sqrt{\beta}}{\sqrt{m}}. \qquad (21.10b)$$

On the other hand, large wave numbers play the main role in the integral in (21.5) for small r. We see from (18.10) that it is then independent of the kind of statistics

$$\mathcal{P}(k,0) \cong -\frac{2me^2}{(2\pi)^7\,\vec{k}^2}\int d^3\vec{k}'\, n^{(0)}(\vec{k}') + O(k^{-4})$$

$$= -\frac{nme^2}{(2\pi)^4\,\vec{k}^2} + O(k^{-4}). \qquad (21.11)$$

Substituting (21.11) into (21.5) we find the asymptotic form of the potential at small distances (in Gaussian units)

$$\tilde{\varphi}(r) = \frac{Ze}{r}e^{-\gamma r}\cos\gamma r\,; \qquad \gamma = 2\left(\frac{\pi mne^2}{\hbar^2}\right)^{\frac{1}{4}}. \qquad (21.12)$$

One can use this formula as long as $r < r_c$. Equation (21.12) replaces the classical Debye law in the region where quantum effects turn out to be important (distances of the same order of magnitude as the de Broglie wavelength, r_c, of the screened charges). More precisely it is valid in the "ultra-quantum" region $r \ll r_c$. We emphasise that (21.11) and (21.12) are independent of the degree of degeneracy of the electron gas; this only determines the limits of their applicability.

An approximation such as (21.4) which is similar to (21.12) can be obtained from (21.5) for small distances, if we use instead of the expansion (21.11) for the polarisation operator a cruder method: we simply drop the second term in the denominator in (21.5), at the same time cutting-off the integral at some upper limit k_0. The latter must satisfy the condition

$$\frac{nme^2}{\hbar^2 k_0^4} \ll 1. \tag{21.13}$$

We then get for the potential a formula such as (21.4) which is suitable for distances $r \lesssim k_0^{-1}$. The parameter k_0 is here, however, not connected at all with the limiting wavenumber k_c. Moreover, it has no clear physical meaning, being merely connected by the inequality (21.13).

We turn now to the case of an arbitrary dispersion law. The expansion of the right-hand side of (18.10) gives for small k

$$\lim_{k\to 0} \mathcal{P}(k,0) = \frac{e^2}{2(2\pi)^7} \lim_{\substack{\eta\to 0 \\ \eta>0}} \mathrm{Re} \int d^4\vec{k}' n^{(0)}(\vec{k}') \frac{n_\alpha n_\beta}{\left(n_\gamma \frac{\partial W(k')}{\partial k'_\gamma} + i\eta\right)^2} \equiv -\frac{e^2}{2(2\pi)^7} b,$$

$$b > 0, \qquad n_\beta = \frac{k'_\beta}{k}; \tag{21 14}$$

and we obtain again (21.6) with

$$r_0^{-1} = \frac{\sqrt{be^2}}{(2\pi)^{\frac{3}{2}}}. \tag{21.15}$$

For $W(\vec{k}) = \vec{k}^2/2m$ (21.15) goes over into (21.8) or (21.9). For the quadratic anisotropic approximation (18.22) we get the same formula, provided we replace m by $(m_1 m_2 m_3)^{\frac{1}{3}}$.

At large k the result depends essentially on the form of $W(\vec{k})$ and can not be written in a general form, unless we cut off the integral in (21.5) at some upper limit and drop the polarisation operator altogether. In that case we get, of course, again (21.4) independently of the form of the energy surfaces.

In how far we can apply in actual fact the asymptotic formulae for $\tilde{\varphi}$ which we have obtained depends, of course, on the specific nature of the problem considered. It is immediately clear that in metals where all distances of any importance are of the order of the lattice constant, neither (21.6) nor (21.12) are strictly valid (forgetting the particular untrustworthiness of the quadratic dispersion law). On the other hand, in semi-conductors the parameter r_c turns out to be about 10^{-6} cm (at room temperature); we can thus find a region where the quantum-mechanical formula (21.12) must be used. We need, however, bear in mind that at distances which are too small (21.12) may turn out to be untenable because the linear approximation (8.17) can not be used. In this approximation we have thus no longer the possibility (which exists in principle) that there are localised plasma oscillations. This fact may narrow the actual region of applicability of (22.12).

One could shew that one can consider the electron-electron interaction in the same way as the electron-external field interaction.

The problem was stated in that way by Bohm and Pines (see, for instance, Pines 1956a, b). Strictly speaking, however, the idea of an electron-electron interaction potential in a solid loses its meaning as this interaction turns out to be retarded due to the exchange of virtual plasmons. We shall consider this problem here in connexion with the case of a totally degenerate fermion gas ($T = 0$). We can then use the usual S-matrix theory (see Appendix I) and introduce an effective interaction matrix

$$U(\vec{x}, \vec{x}') = 2\pi e^2 \int \mathrm{d}^3\vec{k}\, \mathrm{e}^{\mathrm{i}(\vec{k}\cdot\vec{x}-\vec{x}')}\, D_{\mathrm{C}}(\vec{k}, k_0)\Big|_{k_0=\Delta\omega} . \quad (21.16)$$

Here $\Delta\omega$ is the change in the energy of an electron because of its being scattered by another electron. If this change in energy is sufficiently small,

$$\Delta\omega \ll \mu ; \qquad \Delta\omega \ll W(\vec{k}) , \quad (21.17)$$

we have $D(\vec{k}, \Delta\omega) \cong D(\vec{k}, 0)$. In that case (21.16) ceases to depend on the initial and final states of the electrons and can be considered to be the usual interaction potential energy. The right-hand side of (21.16) is then, of course, the same as $e\tilde{\varphi}$, provided we use (21.1) for $\tilde{\varphi}$ and take (21.2) (with $Z = 1$) into account. In particular, if we use the approximation (11.4) for the electron-electron interaction, all conclusions reached in the present section about the interaction between an electron and a point charge will be valid. The case which is characterised by (21.17) is probably of most interest in the theory of metals. The case where finite values of $\Delta\omega$ are important is, however, also possible in principle; in that case it is not possible at all to introduce the concept of an electron-electron interaction (in complete analogy with quantum electrodynamics).

22. DEGENERATE BANDS *

Up to now we have restricted ourselves to the non-degenerate case (in the sense of section 18). Although the method developed here covers a rather large class of problems, it does not enable us to consider a number of systems which are of interest both from a theoretical and from an experimental point of view. We can, namely, not consider any case where we need in the unperturbed problem take into account the dependence of the electron energy not only on the quasi-momentum, but also on some discrete quantum numbers. To this class of systems belong, especially, substances for which:

a. the unperturbed energy values of the charge carriers form degenerate bands (for instance, p-type germanium or silicon);
b. one can not find a clear-cut energy difference between the valence

* Bonch-Bruevich (1958c).

electrons and the electrons in the outer shells (for instance, transition metals);

c. the unperturbed energies of the charge carriers are spin-dependent (ferromagnetics, substances with appreciable spin-orbit interactions); or

d. charge carriers with both positive and negative charges play an important role (semi-conductors and metals with a mixed conductivity).

We shall shew in the present section that one can apply the methods developed earlier to a large extent also to these more complicated cases.

It is well known (Kittel and Mitchell 1954, Luttinger and Kohn 1955, Deĭgen and Pekar 1956) that one can not apply the simple "effective mass method" to the problems enumerated a moment ago: instead of by a single equation with an "effective kinetic energy" $W(-i\nabla_{\vec{x}})$, the unperturbed problem is described by a set of equations

$$\{W_{ab}(\vec{k}) - \delta_{ab} W\} c_b = 0 , \tag{22.1}$$

where W_{ab} is a square matrix while the indices a and b number the different kinds of charge carriers, spin components, and so on (for each given problem we shall thus have, in general, a different set of values for a and b). The eigenvalues of the set (22.1) are the energy eigenvalues for the unperturbed problem, and the wave functions are $c_a e^{i(\vec{k}\cdot\vec{x})}$. We shall number the eigenvalues of (22.1) by an index ν. We have clearly

$$\Sigma_a c_a^+(\nu, \vec{k}) c_a(\nu', \vec{k}) = \Delta(\nu-\nu') , \tag{22.2}$$

$$\Sigma_\nu c_a^+(\nu, \vec{k}) c_b(\nu , \vec{k}) = \delta_{ab} \tag{22.3}$$

It follows furthermore from the general properties of particles moving in a periodic field that W_{ab} and W are even functions of $\vec{k}$.

It is clear that in this case the fermion Green function is a matrix; instead of (18.3) we have

$$G^{(0)}_{c\,ab}(k) = -\frac{1}{(2\pi)^4} \sum_\nu c_a(\nu, \vec{k}) c_b^+(\nu, \vec{k}) \frac{k_0 - W(\nu, \vec{k}) + i\varepsilon[2n^{(0)}(\nu, \vec{k}) - 1]}{[k_0 - W(\nu, \vec{k})]^2 + \varepsilon^2} \tag{22.4}$$

The unperturbed boson Green function retains, on the other hand, its form (18.5) and the polarisation operator is a trace over the indices a and b. If we use as before the improved perturbation theory of section 11 we get for the real part of the polarisation operator

$$\mathrm{Re}\, \mathcal{P}(\vec{k}, \omega) = \frac{2e^2}{(2\pi)^7} \sum_{\nu,\nu'} \int d^3\vec{k}'\, n^{(0)}(\vec{k}', \nu)\, \mathcal{P} \frac{S(\nu, \nu'; \vec{k}', \vec{k})}{W(\vec{k}', \nu) - W(\vec{k}'-\vec{k}, \nu') - \omega} + \frac{S^+(\nu, \nu'; \vec{k}', -\vec{k})}{W(\vec{k}', \nu) - W(\vec{k}'+\vec{k}, \nu') + \omega} . \tag{22.5}$$

Here

$$S(\nu, \nu'; \vec{k}', \vec{k}) = \sum_{a,b} c_a(\nu, \vec{k}')\, c_a^+(\nu', \vec{k}'-\vec{k})\, c_b^+(\nu, \vec{k}')\, c_b(\nu', \vec{k}'-\vec{k}) \ . \quad (22.6)$$

If the crystal has a centre of symmetry, we get, because of the parity of $c_a(\nu, \vec{k})$

$$S(\nu, \nu'; -\vec{k}', \vec{k}) = S(\nu, \nu'; \vec{k}', -\vec{k}) \ .$$

Moreover, it follows from (22.2) that

$$S(\nu, \nu'; \vec{k}', \vec{k})$$

$$= \Delta(\nu-\nu') + [1 - \Delta(\nu,\nu')] \sum_{\substack{n\geq 1 \\ m\geq 1}} k_{i_1} \ldots k_{i_n} k_{j_1} \ldots k_{j_m} A_{i_1 \ldots i_n j_1 \ldots j_m} \cdot \quad (22.7)$$

Here $i_1, \ldots, j_m$ are vector indices and the quantities A are tensors which depend on the structure of the bands in the unperturbed problem. They can easily be evaluated from (22.1), but we do not need these expressions. We merely note that the tensors A contain in their denominators (various powers of) the quantities $\Delta W(\nu, \nu'; \vec{k})$ which are the distances between the ν-th and the ν'-th band for a given quasi-momentum $\vec{k}$. The presence of these functions - which in general are unknown - makes it difficult to use the expressions for A in practical cases.

From (22.7) we have

$$\mathrm{Re}\ \mathcal{P}(\vec{k}, \omega) = \sum_{\nu} \mathrm{Re}\ \mathcal{P}_\nu(\vec{k}, \omega) + \Delta\mathcal{P}(\vec{k}, \omega) \ , \quad (22.8)$$

where $\mathcal{P}_\nu(\vec{k}, \omega)$ is a polarisation operator of the form (18.10) evaluated for the ν-th band and the correction $\Delta\mathcal{P}(\vec{k}, \omega)$ contains terms with $\nu \neq \nu'$.

The first term on the right-hand side of (22.8) is simply the sum of the formally independent contributions from different bands; their mutual interaction manifests itself then only in the definition of the Fermi level. If we neglect the second term, we can transfer all results obtained earlier to the case of degenerate bands simply by summing over ν. This refers, in particular, to the limiting plasma oscillation frequency and to the screening radius. We have thus

$$\omega_0^2 \approx \frac{2e^2}{3\pi^2} \cdot \frac{k_i\, k_j}{\vec{k}^2} \sum_{\nu} \mu_{ij}(\nu) \ . \quad (22.9)$$

To obtain in this approximation the screening radius we must in the right-hand side of (21.15) sum over ν, which should occur now as an index of b.

On the other hand, when we take the term $\Delta\mathcal{P}(\vec{k}, \omega)$ into account we meet with peculiar features which are specific for the degenerate case: the plasma frequencies may be split into several branches and

there may also occur damping which is connected with real interband transitions when the energy of the plasmons is taken into account. The evaluation of these effects is, however, hardly advisable, as the results depend strongly, not only on constants which might be determined empirically, but also on functions such as $\Delta W(\nu, \nu'; \vec{k})$.

Chapter V

CHARGE CARRIERS IN SOLIDS

23. PERFECT SEMI-CONDUCTORS *

We studied in the preceding chapter collective ("plasma") oscillations in solids. We saw that they are essentially caused by the interaction between the electrons: when this interaction vanishes, the corresponding poles of $D_c(k, \omega)$ vanish also. The plasmons clearly obey Bose statistics. We solved thus the second problem stated in section 17: the problem of studying new branches of the energy spectrum of the system (that is, branches which do not occur in the perfect gas) **. In the present section we shall consider the fermion branch of the energy spectrum (that is, the charge carrier spectrum) in a perfect crystal. In that way we shall answer the first problem posed earlier; namely the question of how the interaction changes the "free" particle spectrum. We noted in section 17 that it has a meaning to put the question in that way for semi-conductors, but not for metals. For that reason we shall restrict ourselves to the case of a Boltzmann gas only, and put $n^{(0)}(\vec{k}) = e^{\beta\mu - \beta W(\vec{k})}$ (formally it would be easy to perform all calculations also for a completely degenerate Fermi gas). Furthermore, we shall only consider a system which is not degenerate in the sense of section 18, and moreover use the isotropic approximation $W(\vec{k}) = \vec{k}^2/2m$.

To solve the problem which interests us it is sufficient to evaluate the single-fermion Green function. We use the perturbation theory of section 11, assuming the following two inequalities to hold (we use Gaussian units)

$$\frac{n}{N_{st}} \cdot \frac{e^2}{\hbar v_T} \cdot \frac{1}{\beta\hbar\omega_0} \ll 1 , \qquad \frac{n}{N_{st}} \left(\frac{me^2}{\hbar^2 n^{\frac{1}{3}}}\right)^{\frac{3}{2}} \ll 1 . \tag{23.1}$$

* Bonch-Bruevich (1959a), Bonch-Bruevich and Kogan (1960), Kogan (1959, 1960).

** This solution is, however, not exhaustive. When there are both positive and negative charges (electrons and holes) present the plasma oscillations form only one of the possible boson branches; Mott excitons are another one. It is convenient to study these in the framework of our present theory by using two-fermion Green functions: some of its poles will in the case where we take the interaction into account correspond to bound states of the "electron-hole" system (in that sense the situation is here analogous to the positron problem in quantum electrodynamics).

The first inequality is the important one; the second one is introduced merely to simplify the calculations. For most semi-conductors (23.1) is in actual fact satisfied in a fairly wide range of electron concentrations and temperatures. We remember that we understand by e^2 the square of the charge divided by the dielectric constant of the lattice. This may be very important in homopolar semiconductors (in germanium, for instance, $\varepsilon = 16$). We note also that in a non-degenerate gas we have always by definition

$$\frac{n}{N_{st}} \ll 1 , \qquad n^{(o)}(\vec{k}) \ll 1 . \tag{23.2}$$

In the following we shall, whenever possible, neglect the left-hand sides of (23.2) in comparison with the right-hand sides. Moreover, we can rewrite the first inequality (23.1) in the form

$$\frac{g^2}{\beta\hbar\omega_o} = \beta\hbar\omega_o \ll 1 . \tag{23.3}$$

We may thus assume that $\hbar\omega_o < 2/\beta$, as we shall do in the following.

The general expression (9.5a) for the Fourier transform of the mass operator in the non-relativistic case is now of the form

$$M(k) = -\,i\,e^2 \int d^4k'\, G_c(k')\, \Gamma(k', k)\, D_c(k'-k) , \tag{23.4}$$

where $\Gamma(k', k)$ is the Fourier transform of $\Gamma(x, y; z)$. In first approximation we have

$$M^{(o)}(k) = -\,i\,e^2 \int d^4k'\, G_c^{(o)}(k')\, D_c^{(o)}(k'-k) . \tag{23.4a}$$

From (18.3) and (18.5) we get

$$M^{(o)}(\vec{k}) = -\frac{\beta\omega_o^2}{4(2\pi)^4}\, e^{-\frac{\beta\vec{k}^2}{2m}} \int_0^1 \frac{dx}{\sqrt{x}}\, e^{\frac{\beta\vec{k}^2}{2m}x} . \tag{23.5}$$

In the first non-vanishing approximation the mass operator thus turns out to be real (and, of course, independent of k_o). The imaginary part of the Green function - and also because of (4.9) the spectral function $J(\vec{k}, E)$ - has thus a delta-function form. From (23.5) and (11.1) we get, if we neglect $n^{(o)}(\vec{k})$ as compared to unity,

$$\mathrm{Im}\; G_c(\vec{k}, k_o) = \frac{1}{2(2\pi)^3}\, \delta\left[W(\vec{k}) + (2\pi)^4\, M^{(o)}(\vec{k}) - k_o\right] . \tag{23.6}$$

This means that in the present approximation the interaction leads only to some change ("renormalisation") of the charge carrier energy: this energy is now equal to

$$W_r(\vec{k}) = W(\vec{k}) + (2\pi)^4\, M^{(o)}(\vec{k}) , \tag{23.7}$$

At the same time there is no damping of the quasi-particles and their

momentum distribution function does not change its form. Indeed, it is given by (5.7):

$$f(\vec{k}) = 2(2\pi)^3 \int_{-\infty}^{+\infty} dk_0 \frac{\operatorname{Im} G_c(\vec{k}, k_0)}{e^{-\beta\mu+\beta k_0} - 1} \tag{23.8}$$

Substituting (23.6) into (23.8) we find

$$f(\vec{k}) = e^{\beta\mu-\beta W_r(\vec{k})} . \tag{23.9}$$

As should be the case, the "renormalised" (that is, the observed) electron energy $W_r(\vec{k})$ occurs here.

We note that the right-hand side of (23.6) does nowhere change sign. This is as should be: we saw in section 5 that Im $G_c(\vec{k}, k_0)$ changes sign for $k_0 = \mu$; because of the delta-function character of (23.6) this is possible only if the level of the chemical potential μ falls in the range of $W_r(\vec{k})$ values. This is, however, excluded as we have used the Boltzmann approximation.

It is clear from (23.7) that the interaction may change not only the parameters of the energy spectrum, but also its form: the function $W_r(\vec{k})$ is not a quadratic one. For sufficiently small k we get, when we expand the right-hand side of (23.5) in a power series,

$$W_r(\vec{k}) = \frac{\vec{k}^2}{2m_r} - \tfrac{1}{2} \beta \omega_0^2 , \tag{23.10}$$

where m_r is the "renormalised mass":

$$m_r = m (1 + \tfrac{1}{3} \beta^2 \omega_0^2)^{-1} . \tag{23.11}$$

The second term on the right-hand side of (23.10) gives the renormalisation of the chemical potential

$$\mu_r = \mu - W_r\Big|_{\vec{k}=0} = \mu + \tfrac{1}{2} \beta \omega_0^2 . \tag{23.12}$$

In connexion with the question of the change in the electron spectrum we must draw attention to the following fact. Equations (23.7) and (23.10) describe the change in the electron energy when we take the so-called direct electron-electron interaction into account. We know, however, that the interaction leads also to a screening of the external field, produced by some classical sources. (Indeed, the mass operator occurs in the effective wave equation (9.18) side by side with the screened potential $\tilde{\Phi}$, and not in its stead.) In particular, the regular array of atoms (or ions) of the crystalline lattice which produces the periodic field is a collection of such sources. The field remains, of course, periodic when screening is taken into account, but its precise form is changed, juts as the parameters determining its magnitude are changed. This leads to an additional change in the electron spectrum which is not taken into account in (23.7) and (23.10). These equations give thus, strictly speaking, not yet a complete solution of the problem. In most semi-conductors

this fact is, however, not important. Indeed, in homopolar semi-conductors such as germanium the forces of the interaction between the atoms in the lattice and the electrons are short-ranged, and the screening has no effect upon them for typical (rather large) values of the screening radius: it is clear from (21.1) that $\rho(\vec{k})$ is non-vanishing only for wavevectors comparable with the reciprocal of the range R of the forces; the term including the polarisation operator in the denominator is then small, of the order of $(\gamma R)^4$, where γ is given by (21.12). In ionic semi-conductors this argument is, of course, not valid, but the free charge concentration is then usually so small that a detailed consideration of the screening effects are not of any interest for most problems.

The situation described by (23.6) is very typical for the approximate method of section 11 whenever it is applied to fermion systems with instantaneous interactions. In the first non-vanishing approximation there occurs only a trivial change in the spectrum, and the spectral function retains its delta-function shape. In the higher approximations there occur, as we shall see now, more delicate effects: damping and a change in the distribution function; the analytical structure of the spectral function will therefore also become more complicated: instead of separate poles there occur branch points on the real axis.

Corrections to the mass operator (23.4) may occur by
(i) replacing $G_c^{(0)}(k)$ by an improved expression containing $M^{(0)}(k)$;
(ii) using a more accurate expression for the vertex part; and
(iii) replacing $D_c^{(0)}(k)$ by the more accurate function $D_c(k)$ determined from (11.2).

It is immediately clear that corrections of the first kind contribute to M in order g^4 (or higher order). The same is true of corrections of the second kind, as one can easily verify by direct calculations: when evaluating the corrections of the next approximation to Γ using (9.16), one sees that $\Gamma = 1 + O(g^2)$. On the other hand, replacing $D_c^{(0)}(k)$ by $D_c(k)$ leads to corrections of the order $|g|^3$. Indeed, such a substitution leads to the occurrence of poles at $k_0 = \pm\, \omega_{pl}(\vec{k})$ in the integrand in (23.4) (these poles are encircled in the usual way); the corresponding residue gives a term of order $g^2\omega_{pl}$, that is, of order $|g|^3$. As long as (23.1) is satisfied we can thus restrict ourselves to the corrections of the third kind only. To simplify the calculations we approximate the plasma spectrum by the first term in (18.28) and neglect the damping of the plasma oscillations; we saw in section 20 that this approximation is completely satisfactory in semi-conductors. We find then within the approximation used now by integrating (23.4) over those k-values which are close to the thermal ones

$$\mathrm{Re}\; M(k) \simeq M^{(0)}(\vec{k}) \,, \tag{23.13}$$

$$\operatorname{Im} M(k) = -\frac{me^2\omega_0}{4|k|\hbar(2\pi)^5}\,\theta(k_0+\omega_0)\,\ln\left|\frac{1+\sqrt{2\zeta}}{1-\sqrt{2\zeta}}\right|, \qquad (23.14)$$

where

$$\zeta = \frac{\hbar m(k_0+\omega_0)}{\vec{k}^2}. \qquad (23.15)$$

We have used in (23.14), as in the subsequent equations (23.18) to (23.21), the usual Gaussian units. We note that because of (23.1) and (23.2) Im $M(k) = 0$, if $k_0 = \mu$ (we have normalised the energy here such that $\mu < 0$). In the region of interest to us Im $M(k) \neq 0$, and we get for the imaginary part of the Green function

$$\operatorname{Im} G_c(k) = -\frac{\operatorname{Im} M(k)}{\left[k - W(\vec{k}) - (2\pi)^4 \operatorname{Re} M(k)\right]^2 + \left[(2\pi)^4 \operatorname{Im} M(k)\right]^2}. \qquad (23.16)$$

We can thus easily find the charge carrier momentum distribution function and also the "damping factor" $\gamma(\vec{k})$. We introduce the parameter

$$\rho(\vec{k}) = \tfrac{1}{2}\sqrt{\frac{me^4\beta}{\hbar^2}}\,\frac{1}{kr_D}\,\ln\left|\frac{1+\sqrt{1+\tfrac{1}{3}\beta^2\omega_0^2\hbar^2+\dfrac{\hbar\omega_0}{W(\vec{k})}}}{1-\sqrt{1+\tfrac{1}{3}\beta^2\omega_0^2\hbar^2+\dfrac{\hbar\omega_0}{W(\vec{k})}}}\right|. \qquad (23.17)$$

One must bear in mind the way ρ depends on the charge: as $e^2 \to 0$, ρ tends to zero as $e^2 \ln e^2$. Using (23.8), we get

$$f(\vec{k}) = e^{\beta\mu-\beta W_r(\vec{k})}\left[1+\varphi(\vec{k})\right]. \qquad (23.18)$$

The function $\varphi(\vec{k})$ which describes the quantum corrections to the Boltzmann distribution is given by the equation

$$\varphi(\vec{k}) = -1 + \frac{1}{\pi}\left(\operatorname{Ci}\rho\,\sin\rho - \operatorname{Si}\rho\,\cos\rho + \int_0^{x_m} dx\,\frac{\rho e^x}{x^2+\rho^2}\right), \qquad (23.19)$$

$$x_m = \beta W(\vec{k}),$$

where Ci ρ and Si ρ are the cosine and sine integrals (see, for instance, Whittaker and Watson 1946). As $\rho \to 0$ (vanishing of the interactions), $\varphi(\vec{k}) \to 0$, as should be the case. We get from (23.16) and (23.14) for the damping factor (evaluated according to the prescription of section 4)

$$\gamma(\vec{k}) = \frac{me^2\omega_0}{2k\hbar^2}\,\ln\left|\frac{k+\sqrt{2m\left[W_r(\vec{k})+\hbar\omega_0\right]}}{k-\sqrt{2m\left[W_r(\vec{k})+\hbar\omega_0\right]}}\right| \equiv \frac{k_B T}{\hbar}\,\rho. \qquad (23.20)$$

In the most interesting region where $k \sim \sqrt{mk_BT}/\hbar$ this leads to

$$\gamma \cong \frac{me^2\omega_0}{2k\hbar^2} \ln \frac{12}{\beta^2 \hbar^2 \omega_0^2} \tag{23.21}$$

We note that the value of γ may turn out to be not too small notwithstanding the smallness of the parameters in (23.1).

We see thus that if we use the spectral theorems of sections 4 and 5 combined with the "iterative" perturbation theory of section 11, we are able to obtain expressions which go beyond the bounds of the simple expansions in powers of the coupling constant. A similar situation occurs also in quantum electrodynamics (compare Bogolyubov, Logunov, and Shirkov 1959). In the language of the diagram technique method (see appendix I) one might say that the methods developed here sum at once the most important Feynman diagrams.

We note, however, that in the case considered the problem contains several dimensionless parameters and a formal expansion in terms of these may turn out to be insufficient: higher order terms in the expansion may turn out to be just as important as earlier ones. There can, for instance, occur purely classical terms proportional to the Debye parameter $\beta e^2 n^{1/3}$. The question as to the true structure of the perturbation theory series can be solved here, as in other similar cases, by using methods such as the renormalisation group method; so far this problem has not yet been considered in connexion with the present problem.

24. IMPERFECT METALS

In the present and the next section we outline a possible way of solving another of the problems stated earlier (see section 17): what is the influence of defects on the electron energy spectrum in solids We shall assume here that we know the charge carrier spectrum in the perfect crystal.

It is clear that for the present we can only qualitatively study the spectrum. Indeed, because of the strong screening (screening radius of the order of k_F^{-1}) the main role is played by the field near the defects and in that region all detailed (and as a rule unknown) peculiar features of the structure of the microfield in the crystal will be important. Bearing this in mind we shall consider the simplest model where hydrogen-like atoms in solution in the lattice (or adsorbed onto the surface) play the role of defects. The problem then consists in studying the change in energy and in energy density in the system when one electron is added to it (under conservation of the neutrality condition). We know that to do this it is sufficient to find the single-fermion Green function $G_c(x, x')$ when there is a field present which is created by the structural defects. Its poles determine the required energy changes and its limiting form when $x_0' \to x_0$

* Bonch-Bruevich and Glasko 1958, 1959.

($x_0' > x_0$) gives us the matrix elements of the "single-particle" density matrix.

To evaluate the poles of the Green function we use the effective wave equation (9.18). In the case considered it has the form

$$W(-i\nabla_{\vec{x}})\,\chi(\vec{x}) - \mu\,\chi(\vec{x}) + \int d^3\vec{x}'\, M(\vec{x},\vec{x}';E)\,\chi(\vec{x}') + e\,\tilde{\varphi}(\vec{x})\,\chi(\vec{x}) = E\chi(\vec{x})\,. \tag{24.1}$$

where $\tilde{\varphi}(\vec{x})$ is the potential of the field created by the defects. For the sake of simplicity we have dropped the possible matrix indices of W, M, and χ. Everything in the present section refers equally well to the degenerate band case.

One must bear in mind that depending on the problem considered W may contain an additive constant which is connected with the energy of the atom far from the metal (this occurs, for instance, in the case of chemical adsorption). Whether or not this constant is present does not alter the following discussion at all.

We noted already in section 9 that the eigenvalue problem connected with (24.1) is in general non-Hermitean: the mass operator may contain a "non-Hermitean" part. We shall, however, see that for our discussions we are especially interested in the case when $\mathrm{Re}\,E \cong 0$ (Fermi surface). We shewed in section 5 that the imaginary part of the single-fermion Green function then vanishes (the same is therefore also true of the imaginary part of the mass operator). We shall accordingly consider (24.1) as a normal Hermitean eigenvalue problem bearing in mind that the results obtained in this way will, strictly speaking, be true only as $E \to 0$.

Formally we can "Hermiteise" (24.1) by replacing $M(\vec{x},\vec{x}';E)$ by $M(\vec{x},\vec{x}';0)$. We can then combine the first three terms on the left-hand side of (24.1) into one operator W_r:

$$W_r\chi(\vec{x}) = W(-i\nabla_{\vec{x}})\,\chi(\vec{x}) - \mu\,\chi(\vec{x}) + \int d^3\vec{x}'\, M(\vec{x},\vec{x}';0)\,\chi(\vec{x}')\,, \tag{24.2}$$

and (24.1) becomes

$$W_r\,\chi(\vec{x}) + e\,\tilde{\varphi}(\vec{x})\,\chi(\vec{x}) = E\,\chi(\vec{x})\,. \tag{24.3}$$

The operator W_r is an integral operator, or a differential operator of infinite order, which comes to the same. This is, however, also true of the initial operator W so that in that respect we have not introduced any new difficulties. It is clear that the eigenvalues of W_r at once determine the spectrum of the charge carriers in the perfect lattice (near the Fermi surface). The form of the Fermi surface (which can be determined experimentally) is, in particular, given by the equation

$$W_r(\vec{k}) \equiv W(\vec{k}) + (2\pi)^4\, M(\vec{k},0) - \mu = 0\,, \tag{24.4}$$

where $\vec{k}$ is the quasi-wavevector of the charge carriers.

We shall first of all consider a low impurity concentration when the effects produced by separate atoms are additive, and the potential in (24.3) can be connected with a single atom. In the case considered this potential is defined by (21.1) and (21.2) with $Z = 1$, while the precise form of the polarisation operator is immaterial for us. Equation (24.3) has then, in general, two classes of solutions corresponding to the continuous and to the discrete spectrum. In the first case the influence of the impurity atoms is only to change the distribution of the electron density inappreciably, as long as the defect concentration is small. There is then no localisation of electrons near the impurity centres. These solutions describe the normal fermion branch of the spectrum in the metal considered; the corresponding eigenvalues are for sufficiently small impurity concentrations simply given by $W_{\mathbf{r}}(\vec{k})$ (this is connected with the statement that one can determine its form experimentally).

Solutions of the second class describe non-uniform electron distributions with a maximum near the structural defect. In that sense one can call the corresponding energy values localised levels *; one must, however, bear in mind that, as we noted in section 9, these are not "single-electron" levels in the literal sense of the word. It is clear that if these states exist, they are energetically more favourable than the solutions of the first kind (if we reckon the energy from the Fermi surface we have $E > 0$ in the first case, and $E < 0$ in the second case). It is extremely important, however, that - independent of the approximation used - the potential $\tilde{\varphi}$ in (24.3) is always screened with a screening radius $\sim k_F^{-1}$ ($\sim 10^{-8}$ cm as we are dealing with a metal). This means that depending on the parameters of the problem considered there may well be no solutions of the second kind. In that case the atoms included in the lattice (or adsorbed onto the surface) will inevitably be ionised. The question of whether or not there are "localised" solutions can be clarified by studying (24.3) as $E \to 0$, and just in this case is the replacement of $M(\vec{x}, \vec{x}'; E)$ by $M(\vec{x}, \vec{x}'; 0)$ justified.

We must emphasise that the general conclusion about the possible existence of two kinds of electron states in an imperfect metal is not at all connected with the previously made special assumptions about the nature of the included impurities. It is essential only that we are dealing with structural defects of a "localised" character. In particular, the discussion given here refers also to the energy spectrum of a not completely ordered alloy where the irregular distribution of one of the components plays the role of the structural defects.

The inclusion of impurities which do not create localised levels leads to an increase in the concentration of free charge carriers. In

* They are the many-electron analogue of the localised levels of the standard single-electron semi-conductor theory. To avoid misunderstandings we note that the presence of such states does not contradict the Pauli principle at all, as the continuous spectrum is, strictly speaking, not described by plane waves, but by the solutions of (24.3).

the temperature range where scattering by lattice vibrations dominates this can lead to a specific influence of the impurities on the electrical conductivity of the substance: this will not decrease but increase somewhat (proportionally to the increased carrier concentration).

All metals with reference to a given kind of structural microdefects (or all microdefects with reference to a given metal) can thus be divided into two classes corresponding to the presence or absence of localised states.

One must emphasise, however, that this division into two classes, defined by the parameters of the problem, is not at all an absolute one. When the electron concentration in the metal is changed (when the atomic composition of the alloy is changed) a system may go from one class into the other. Experimentally this may reveal itself in a change of the way the impurities influence the electrical conductivity or, if we are dealing with adsorbed atoms, in the specific dependence of the heat of adsorption on the composition of the (adsorbent) alloy.

We turn now to systems with a larger impurity concentration when it is no longer clear from the outset that the effects caused by the separate atoms are additive. The function $\tilde{\varphi}(\vec{x})$ is in that case a sum of screened potentials φ_a and we have a "molecular" problem. In the case of most interest when there are localised levels present we can use the well-known methods of quantum chemistry and write (24.3) in the form

$$\chi(\vec{x}) = \Sigma_i c_i \chi_a(\vec{x}-\vec{R}_i) , \tag{24.5}$$

where i numbers the impurity atoms whose radius vectors are $\vec{R}_i$, c_i are coefficients which must be evaluated, and the $\chi_a(\vec{x}-\vec{R}_i)$ are the eigenfunctions of the "atomic" problem which are evaluated by neglecting in (24.3) the potentials of all atoms bar the i-th one. The sum in (24.5) is over all impurity atoms (or other structural defects of an "atomic" type). One obtains for the c_i the usual set of equations (E and E_a denote respectively the eigenvalues of the "molecular" and the "atomic" problems)

$$\Sigma_i c_i \{(E-E_a) S_{ik} + V_{ik}\} = 0 , \quad k = 1,2,\ldots \tag{24.6}$$

Here

$$S_{ik} = \int \chi_a^+(\vec{x}-\vec{R}_k) \chi_a(\vec{x}-\vec{R}_i) \, d^3\vec{x} , \tag{24.7}$$

$$V_{ik} = \sum_{j\neq i} \int \chi_a^+(\vec{x}-\vec{R}_k) \tilde{\varphi}_a(\vec{x}-\vec{R}_j) \chi_a(\vec{x}-\vec{R}_i) \, d^3\vec{x} . \tag{24.8}$$

We see at once that the dimensions of the "region of localisation" of the χ_a are of the order of the screening radius (or even less). We saw in section 21 that at distances which are a few times larger than the lattice constant the "atomic" potential is with fair accuracy given by (21.6), (21.7), and (21.15). From this it follows that the quantities S_{ik} and V_{ik} with $i \neq k$ are exponentially small, that is,

$$E = E_a \{1 + O(e^{-d/r_0})\} . \tag{24.9}$$

Here d is the average distance between impurities and r_0, as always, the screening radius.

It thus turns out that practically always the impurity concentration turns out to be "sufficiently small" (in the sense of the conditions stated above), as soon as one can speak about impurities in the given metal (it is clear that if the average distance between the impurity atoms approaches the lattice constant, the concept of structural microdefects loses any meaning and we must talk about the formation of a mixed phase). The reason for this is very clear: the influence of a given structural defect is limited to its immediate vicinity with linear dimensions of the order of the screening radius, that is, (in a metal) of the order of the lattice constant. When we apply this to the theory of chemical adsorption this means that there are practically no "boundary" layer effects in a metal (Vol'kenshteĭn and Sandomirskiĭ 1955, Engell 1954). We emphasise, however, that we are dealing here with metals with an ideally pure surface, in particular without semi-conducting films. The presence of the latter may distort the situation completely.

The considerations given here enable us to extend immediately to metals a number of qualitative results obtained earlier by different authors in the electron theory of chemisorption and catalysis in semiconductors (see, for instance, the survey by Vol'kenshteĭn, 1953a). If, thus, it is possible that there exist localised states in a given metal, it has a meaning to apply to this metal the whole phenomenological theory of the formation of a adsorbed layer bound to the adsorbent. One must, however, draw attention to the following facts:

Firstly, we are talking here about transferring to the case of a metal only some of the phenomenological concepts of the electron theory of adsorption and catalysis in semi-conductors, but not by any means its methods of calculating.

Secondly, the statistics of the occupation of the localised levels turns in the present case to be considerably simpler than in semiconductors: because of the high concentration of free electrons in a metal the Fermi level is practically fixed in metals and the effects of an "interaction through the electron gas" (Vol'kenshteĭn 1953b) which is characteristic for semi-conductors is here completely absent. In this respect metals, and not semi-conductors, resemble most closely the classical adsorbent of the Langmuir theory.

We emphasise that in none of the discussion of the present section we introduced model approximations or made any special assumptions. We used only two statements: that it is possible to state the problem in the "single-quasi-particle" form (24. 1) and that the impurity potential occurring in (24. 1) is strongly screened. The first is, however, a consequence of the spectral properties of the Green functions (section 9), while the second follows immediately from dimensional considerations.

25. LOCALISED LEVELS IN SEMI-CONDUCTORS *

The general method of section 24 can, of course, also be applied to semi-conductors. There are here, however, some peculiarities which enable us to obtain in a number of cases also quantitative solutions of the problem of localised levels.

First of all, the screening radius is in semi-conductors, as a rule, very large compared to the lattice constant independently whether it is determined from (21.7) or from (22.12). This enables us under well-defined conditions to use the effective mass method in one of its standard forms, by approximating $W(\vec{k})$ by (18.22) (or the appropriate matrix generalisation, see section 22). This can be done in the theory of the shallow localised (so-called hydrogen-like) levels formed, for instance, by elements of the third or fifth group in germanium and silicon.

Secondly, we saw in section 23 that we can evaluate explicitly the mass operator M in a rather wide range of charge carrier concentrations and temperatures; its imaginary part turns then, indeed, out to be small compared to its real part, and the Hermitean problem (24.3) has a meaning beyond $E = 0$. The usual theory of localised levels in semi-conductors is obtained from (24.3) if we neglect both the mass operator and the screening.

Taking screening into account in the theory of localised levels is important not only (and not so much) from a purely quantitative point of view, but rather from the point of view of principles. Indeed, the screening radius depends, from (21.7) and (21.12), on the free charge concentration and on the temperature. The latter occurs also, implicitly, in (21.12) as the concentration n depends on it. This means (in complete accordance with the general discussion of section 16) that the ionisation energy of an impurity in semi-conductors is not a purely mechanical, but a thermodynamic quantity. The same is, clearly, also true of the excitation energies (if there are excited impurity states as well as a ground state), of the number of levels created by given structural defects, and in general of all characteristic impurity states without exception: they depend on T and n, that is on the position of the Fermi level in the crystal (in particular, also on the concentration both of given and of strange impurities). It is thus possible by changing T and n to manipulate the semi-conductor energy spectrum in a known manner. It is here important that both the equilibrium and the non-equilibrium charge carriers play a role in the screening. Indeed, the mean free flight time of the latter is determined by recombination processes, while the screening, on the other hand, is fully established as soon as an equilibrium distribution of free charges has been established (for a given total number of free charges) and a static value of the field has been reached. The first

* Bonch-Bruevich 1959d.

of these processes is characterised by the mean flight time and the second by the Maxwell relaxation time. Both these parameters are as a rule several orders of magnitude smaller than the recombination life time and that is the basis of our statement: the non-equilibrium carriers have plenty of time to take part in the screening before they recombine. This means that the concentration of screened charges can be changed independently of the impurity concentration in the sample: by injection.

We emphasise that it is in principle possible to manipulate not only the distribution of localised levels but also their total number and even their existence itself: if the screening radius is sufficiently small the localised electron states may vanish completely (compare section 24). The experimental vanishing of the localised excited and ground states could manifest itself, for instance, in the vanishing of the infrared impurity absorption when the free charge carrier concentration is changed.

To estimate the corresponding critical values of T and n it is necessary to solve (24.3) explicitly for some specific case. We shall consider here the simplest case of a "hydrogen-like" model, assuming the bands to be non-degenerate, neglecting the anisotropy of the effective mass tensor, and considering the core of the impurity atom simply as a point charge. This is, of course, a rather approximate way of posing the problem; there is therefore no point in evaluating the (relatively small) corrections to the mass operator in (24.3). We shall use here (21.12) as the impurity potential $\tilde{\varphi}(\vec{x})$. Indeed, we are clearly most interested in this problem in distances of the order of the Bohr radius in the crystal, $\hbar^2/me^2$; this distance is as a rule, for typical values of the effective mass and of the dielectric constant, considerably smaller than the average de Broglie wavelength.

The problem is thus reduced to finding the solution of the usual Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\chi - \frac{e^2}{r}e^{-\gamma r}\cos(\gamma r)\chi = \lambda\chi . \qquad (25.1)$$

The eigenvalue λ differs from E because of our choice of the energy zero: the energy is reckoned in (25.1) from the bottom of the conduction band and the absolute value of the energy of the lowest level, $|\lambda_{\min}|$, is thus immediately the ionisation energy, J. To fix our ideas we consider here, as always in this book, the case of an n-type semi-conductor. Changing our results to apply to a p-type sample (within the frame work of the approximations made here) is straightforward.

If γ is small (weak screening) we can use standard perturbation theory, choosing as the unperturbed problem an equation such as (25.1) with a purely Coulomb interaction potential (this is clearly nothing but the case of very low carrier concentrations considered in the standard theory; in that case screening plays no role). In first

approximation we get for the change in the ionisation energy as compared with the pure "hydrogen" case (in Gaussian units)

$$\Delta J = \hbar\omega_0 = \sqrt{\frac{4\pi ne^2\hbar^2}{m}}. \tag{25.2}$$

As we noted earlier, the dependence of the ionisation energy on the electron concentration involves a corresponding dependence on the impurity concentration. This fact has been observed long ago experimentally (see, for instance, Pearson and Bardeen 1949). We must, however, bear in mind that this dependence may be caused by a whole number of different causes which are not necessarily connected with screening; a comparison of the consequences of (25.2) with experimental data is thus for the present still premature.

If we wish to use perturbation theory we can use (25.2) only as long as $\Delta J/J$ is sufficiently small. When the screening becomes stronger we must solve (25.1) numerically. A detailed description of a method for doing this can be found in a paper by Bonch-Bruevich and Glasko (1958). We give here only the critical value of the concentration n_c when the ionisation energy vanishes:

$$n_c = \frac{8}{3\pi^2}\left(\frac{me^2}{\hbar^2}\right)^3. \tag{25.3}$$

The factor $8/3\pi^2$ arises from a difference in notation in the present book and in the paper by Bonch-Bruevich and Glasko.

We note in conclusion that the possibility that the localised levels vanish forces us to reappraise anew the theory of the metallic conduction of semi-conductors based upon this idea (Davydov and Shmushkevich 1940) which was rejected originally because of arguments connected with the Coulomb character of the impurity potential. (This is, of course, not an objection against another possible explanation of the metallic conduction which is based upon the impurity band concept: Pekar and Krivoglaz 1952).

26. THE ELECTRON-PHONON COUPLING CONSTANT IN METALS *

One possible application of the general theory of screening developed in section 21 is the problem of the interaction between the charge carriers and the phonons in a metal. Indeed, this interaction is basically nothing but the interaction between the electrons and an additional electrical field produced when the ions are displaced from their equilibrium positions **. This was the way the problem was put by Bardeen (1937), Overhauser (1953), and Bardeen and Pines

* Bonch-Bruevich (1959e).

** There is also a magnetic correction (Overhauser 1953), but this is clearly much less important.

(1955). The problem consists here only in taking the screening of the free charge field properly into account.

In the papers mentioned above the screening effect was taken into account either by the Thomas-Fermi method, or in the self-consistent field approximation, or, finally, by using the redundant variable method. There are, however, serious doubts whether one can apply the first method to solids, as it is essential a semi-classical method; the self-consistent field approximation is in metals also connected with a number of mathematical difficulties (see, for instance, Pekar 1948); finally, we shewed in section 21 that the screening is taken into account only approximately in the redundant variable method. We shall see that the Green function method enables us to give in principle an exact solution of the problem as soon as we know the charge carrier dispersion law in a perfect lattice.

We shall consider for the sake of simplicity a lattice with one atom in the elementary cell. As we are interested only in long wavelength effects we can consider the ions to be point particles.

We shall denote the displacement vector of an ion from its equilibrium position by $\vec{u}(\vec{x})$. The additional charge density arising from such a displacement is

$$\delta\rho = Ne \operatorname{div} \vec{u} , \tag{26.1}$$

where N is the ion concentration. An additional electron potential energy

$$U = - e\,\tilde{\varphi} , \tag{26.2}$$

corresponds to a given value of $\delta\rho$, and the screened potential $\tilde{\varphi}$ is given by (21.1). We emphasise that we are not interested here in any assumption about the form of the polarisation operator. The approximation $\Gamma = 1$ in the long wavelength region is justified as it means only the neglect of the small "spread" of the electron.

We use the usual expression for the displacement vector:

$$\vec{u}(\vec{x}) = \sum_{\vec{k},\nu} [2d\omega(\vec{k},\nu)V]^{-\frac{1}{2}} \{\vec{\varepsilon}(\vec{k},\nu)\, e^{i(\vec{k}\cdot\vec{x})-i\omega t}\, \xi(\vec{k},\nu) + \text{Herm. conj.}\} . \tag{26.3}$$

Here V is the fundamental volume, d the crystal density, $\vec{k}$ and ω the phonon wavevector and frequency, $\nu = 1, 2, 3$ enumerates the vibration branches ($\nu = 1$ corresponds to the longitudinal branch), $\vec{\varepsilon}(\vec{k},\nu)$ the displacement unit vector, and ξ and ξ^+ are the phonon annihilation and creation boson operators. Substituting (26.3) into (26.1) and using (11.2), we get

$$U = - \frac{iNe^2}{\sqrt{V}} \sum_{\vec{k}} \frac{|\vec{k}|}{\sqrt{2d\omega(\vec{k},1)}} \cdot \frac{1}{\vec{k}^2 - (2\pi)^4\, \mathcal{P}(\vec{k},\omega(\vec{k})) + i\varepsilon}$$
$$\times \{e^{i(\vec{k}\cdot\vec{x})-i\omega(\vec{k},1)x_0}\, \xi(\vec{k},1) - \text{Herm. conj.}\} . \tag{26.4}$$

We saw in section (18) that the real roots of the equation

$$\vec{k}^2 - (2\pi)^4 \mathcal{P}(\vec{k}, \omega) = 0$$

are connected with the plasma waves. Their frequencies are in a metal much larger than sound frequencies and the denominator in (26.4) will thus not vanish. Moreover, as the phonon energies are small compared with the Fermi energy we can replace the polarisation operator by its value for $\omega = 0$. (We saw in section 11 that in fact only the ratio of ω and μ enters into $\mathcal{P}$ but not these quantities separately.)

Furthermore, in the long wavelength region (which is the only one of interest, for instance, in the theory of electrical conductivity) we can neglect $\vec{k}^2$ compared to $|\mathcal{P}(\vec{k}, 0)|$ and we may assume the phonon spectrum to be the Debye spectrum: $\omega(\vec{k}, 1) = ck$; if we use (21.14) we can thus finally obtain the standard formula *

$$U = -iG \sum_{\vec{k}} \sqrt{\frac{2\omega(\vec{k},1)}{V}} \{e^{i(\vec{k}\cdot\vec{x})-i\omega(\vec{k},1)x_0} \xi(\vec{k},1) - \text{Herm.conj.}\}\ , \quad (26.5)$$

where the dimensionless coupling constant G (in the usual Gaussian units) is given by

$$G = \frac{(2\pi)^3 N \hbar \sqrt{z}}{\sqrt{M\mu}\, c\, b}\ . \quad (26.6)$$

Here z is the effective number of electrons per atom, M the ion mass in the lattice, and μ the Fermi energy. In particular, in the quadratic isotropic approximation which is usually employed in problems involving electron-phonon interactions we get

$$G = \frac{\sqrt{2}}{z^{\frac{1}{6}}} \left(\frac{\pi}{3}\right)^{\frac{2}{3}} \frac{\hbar}{mc} N^{\frac{1}{3}} \left(\frac{m}{M}\right)^{\frac{1}{2}}\ . \quad (26.7)$$

This quantity is apparently equal to about 0.3 to 0.4.

We note that in (26.6) only the value of the polarisation operator at $k_0 = k = 0$ occurs. We shewed in section 11 that one can evaluate this quantity very accurately. Possible inaccuracies of (26.7) can thus not be connected with the fact that we took screening into account, but only with the phonon or charge carrier dispersion laws. In a real metal the latter is usually not evaluated in the simple quadratic approximation (let alone the isotropic approximation) and has a much more complicated form. In this connexion it is useful to point to the connexion of G with the screening radius of the static field of the free charges. We have from (21.15) (for any dispersion law for the electrons)

* We emphasise that none of these approximations are necessary; they were introduced to get the same result as the one usually obtained.

$$G = \frac{4\pi N \sqrt{z}\, e^2\, r_0^2}{\sqrt{M\mu}\, c}. \tag{26.8}$$

The reason for this connexion is very clear: as the phonon frequencies are small compared with the Fermi frequency the additional field connected with the lattice vibrations acts practically as a static field on the charge carriers.

It is relevant to draw attention to the fact that in the framework of the method developed here, the derivation of (26.8) is practically trivial. This illustrates (just like the contents of section 24) the possibility of a semi-phenomenological approach in the framework of the Green function method.

Chapter VI

ELECTRON-PHONON INTERACTION

27. PERTURBATION THEORY *

Until relatively recently the interaction between charge carriers and lattice vibrations was considered only in connexion with the theory of non-equilibrium processes such as electrical conductivity. One assumed that the charge carrier energy spectrum was "formed" under the influence of the strong interaction between the carriers and the field of the perfect lattice and perhaps of the carriers with one another; the lattice vibrations, however, only acted as a source for the rare transitions between the electron states in the perfect crystal. Gradually, however, it was found that for a number of cases such a way of stating the problem would be insufficient and that one should take the interaction with the phonons explicitly into account already when determining the energy spectrum of the system.

Firstly, this interaction is not at all small in any sense in a number of crystals (Pekar 1946a, 1951; Bogolyubov 1950; Tyablikov 1951a). Taking this into account already in the evaluation of the energy spectrum of the system led to the concept of a special kind of charge carriers in ionic crystals: electrons moving together with a polarisation cloud generated by them. Elementary excitations of this kind were called polarons (Pekar 1946a).

Secondly, it was found that in a metal the electron-phonon interaction, even though it may be relatively weak, may lead to a radical change in the charge carrier spectrum: it is the cause of superconductivity (Fröhlich 1950, Bardeen, Cooper, and Schrieffer 1957a, b, Bogolyubov 1958). This case is also of great methodological interest: we have here a very clear example of the fact that even a weak interaction between fermions and a quantum field can lead to effects which as a matter of principle can not be evaluated within the perturbation theory framework and which are described by non-analytical functions of the coupling constant.

Thirdly, it was found (Radkowsky 1947, Fan 1951, Tyablikov 1951b) that the electron-phonon interaction leads in homopolar semiconductors to a temperature dependence of the width of the forbidden band, the ionisation energy of localised levels, and so on (even though it may not be able to explain this dependence completely).

In the present section we shall study the interaction between the

* Bogolyubov and Tyablikov (1959), Bonch-Bruevich (1960).

electrons and the acoustic phonons in the framework of the perturbation theory of section 11 (without the renormalisation group). Although this approximation does not take superconductivity effects into account, it is sufficient for a number of problems.

We use the simplest isotropic approximation for the unperturbed electron spectrum, and put

$$W(p) = \frac{\vec{p}^2}{2m} . \tag{27.1}$$

We shall in accordance with this also assume the electron-phonon interaction to be isotropic and describe it by the Hamiltonian (6.17) with the field function (6.16).

We evaluate first of all the Green function for the free phonon field $D_C^{(0)}(k)$ *. We denote by $\nu(\vec{k})$ the average number of phonons ** (averaged over the unperturbed ensemble) with wavevectors k:

$$\nu(\vec{k}) = \langle \xi^+(\vec{k})\, \xi(\vec{k}) \rangle_0 .$$

We denote the phonon frequency, as in section 6, by $\omega(k)$. We have clearly

$$\nu(\vec{k}) = \frac{1}{e^{\beta\omega(\vec{k})} - 1} . \tag{27.2}$$

We note that $\omega(\vec{k})$ is an even function. We shall in the following use for small wavenumbers the isotropic Debye approximation

$$\omega(\vec{k}) = ck , \qquad k = |\vec{k}| . \tag{27.3}$$

The constant c is the "bare" sound velocity, that is, the one which would be observed, if there were no interaction with the charge carriers. From (6.16) and (7.11) we get

$$\begin{aligned} D_C^{(0)}(x,x') &= -\,i \langle T\{\Phi(x)\, \Phi(x')\} \rangle \\ &= -\frac{i}{2(2\pi)^3} \int d^3\vec{k}\, \frac{\vec{k}^2}{\omega(\vec{k})}\, e^{i(\vec{k}\cdot\vec{x} - \vec{x}')} \{[\nu(\vec{k})+1]\, e^{-i\omega(\vec{k})|x_0 - x_0'|} \\ &\quad + \nu(\vec{k})\, e^{i\omega(\vec{k})|x_0 - x_0'|}\} \end{aligned} \tag{27.4}$$

The integral is here over the first (phonon) Brillouin zone. In the following we shall indicate this by a bar over the integral sign. It is convenient to express $D_C^{(0)}(x, x')$ as a four-dimensional Fourier integral. To do this we use a relation which we easily verify to be correct:

* In the present chapter we shall not consider effects connected with the Coulomb interaction; the fact that we use for the phonon Green function the same notation as was used for the photon Green function in chapter IV can thus not lead to any misunderstandings.

** We are dealing here with phonons of the acoustical longitudinal branch, in accordance with the problem considered.

$$\int_{-\infty}^{+\infty} dk_0 \frac{e^{-ik_0(x_0-x_0')}}{k_0^2 - \omega^2(\vec{k}) \pm i\epsilon \cdot \omega(\vec{k})} = \mp \frac{\pi i}{\omega(\vec{k})} e^{\mp i\omega(\vec{k})|x_0-x_0'|} . \qquad (27.5)$$

Using (27.5) we can write (27.4) as follows

$$D_c^{(0)}(x, x') = \int d^4k \, e^{-i(k, x-x')} \, D_c^{(0)}(k) , \qquad (27.6)$$

$$D_c^{(0)}(k) = \frac{\vec{k}^2}{(2\pi)^4} \frac{k_0^2 - \omega^2(\vec{k}) - i\epsilon [2v(\vec{k}) + 1]}{[k_0^2 - \omega^2(\vec{k})]^2 + \epsilon^2} . \qquad (27.7)$$

In particular we have

$$\text{Im } D_c^{(0)}(k) = - \frac{\vec{k}^2}{(2\pi)^4} [2v(\vec{k}) + 1] \, \delta [k_0^2 - \omega^2(\vec{k})] . \qquad (27.8)$$

This function has a delta-function singularity at $|k_0| = \omega(\vec{k})$, as should be the case (compare section 4).

As before, we take (5.20) for the unperturbed single-electron Green function. This means, in particular, that we consider charge carriers in one band only. The polarisation operator of such a system has in the first non-vanishing approximation in the coupling constant the same form as in chapter IV: we only need replace in the expressions obtained there the electron charge e by the coupling constant g. We obtained this coupling constant for metals in section 26, and for homopolar semi-conductors it is given by the equation

$$g = E_c^{(1)} \sqrt{\frac{\hbar}{d}},$$

where d is the density in the crystal and $E_c^{(1)}$ the deformation potential constant (see Shockley 1953, Pekar and Deĭgen 1951).

Using (11.2) we get thus for the phonon Green function, if we take the electron-phonon interaction into account,

$$D_c(k) = \frac{\vec{k}^2}{(2\pi)^4} \frac{k_0^2 - \omega^2(\vec{k}) - i\epsilon [2v(\vec{k}) + 1]}{[k_0^2 - \omega^2(\vec{k})]^2 + \epsilon^2 - (2\pi)^4 \vec{k}^2 \mathcal{P}^{(0)}(k) [k_0^2 - \omega^2(\vec{k}) - i\epsilon(2v+1)]} \qquad (27.9)$$

The real part of the polarisation operator is for real $k_0 \equiv \omega'$ given by

$$\text{Re } \mathcal{P}^{(0)}(\vec{k}, k_0) = \frac{2mg^2}{(2\pi)^6 k} \int_{-\infty}^{+\infty} dk' \, k' \, n^{(0)}(k') \, \mathcal{P} \ln \left| \frac{(k' - \frac{k}{2})^2 - \frac{m^2 k_0^2}{k^2}}{(k' + \frac{k}{2})^2 - \frac{m^2 k_0^2}{k^2}} \right| . \qquad (27.10)$$

For the imaginary part we find

$$\operatorname{Im} \mathcal{P}^{(0)}(\vec{k}, k_0) = \frac{ng^2 \sqrt{2\beta m}}{8(2\pi)^3 \, k \, F_{\frac{1}{2}}(\beta\mu)} \ln \frac{1 + \exp\left\{\beta\mu - \dfrac{\beta k^2}{8m}\left(1 - \dfrac{2m\omega'}{k^2}\right)^2\right\}}{1 + \exp\left\{\beta\mu - \dfrac{\beta k^2}{8m}\left(1 + \dfrac{2m\omega'}{k^2}\right)^2\right\}}, \tag{27.11}$$

where

$$F_\zeta(\beta\mu) = \int_0^\infty \frac{x^\zeta \, dx}{e^{x-\beta\mu} + 1}; \qquad k_0 = \omega' - i\gamma, \qquad \gamma \to 0, \qquad \gamma > 0.$$

We know that if the system is not completely degenerate, the right-hand side of (27.11) is non-vanishing for any k, and we can at once take in (27.9) the limit $\epsilon \to 0$.

We can, in principle, study the spectrum of the phonons interacting with the electrons in the same way as we studied the plasma spectrum in sections 18 to 22. If we assume that the damping of the phonons is sufficiently small, we get the following dispersion relation to determine the frequency (k_0 real)

$$k_0^2 - \omega^2(\vec{k}) - (2\pi)^4 \vec{k}^2 \operatorname{Re} \mathcal{P}^{(0)}(\vec{k}, k_0) = 0. \tag{27.12}$$

We restrict ourselves to the small k region and we use the approximation (27.3). An investigation shews that, in contradistinction to (18.7), (27.12) does not have roots $k_0(\vec{k})$ which remain finite as $\vec{k} \to 0$. This should, of course, be the situation: the spectrum of actual acoustical phonons should start at zero. We would have obtained the same for a more complicated dependence $\omega(\vec{k})$; the only essential condition is that $\omega(\vec{k}) \to 0$ as $\vec{k} \to 0$. In accordance with this we put

$$k_0^2(\vec{k}) = c_r^2 \, k^2, \tag{27.13}$$

where c_r is the "renormalised" (that is, the actually observed) sound velocity. The right-hand side of (27.10) tends then for small k to a constant

$$\lim_{\substack{\vec{k}\to 0 \\ k_0 = c_r k}} \operatorname{Re} \mathcal{P}(\vec{k}, k_0) = -\frac{4mg^2}{(2\pi)^6} \int_0^\infty \mathcal{P} \frac{k'^2 \, dk'}{k'^2 - m^2 c_r^2} n^{(0)}(k'), \tag{27.14}$$

which shews the justification of the assumption (27.13). Substituting (27.13) and (27.14) into (27.12) we get an equation to determine the observed sound velocity for any degree of degeneracy of the electron gas:

$$c_r^2 + \frac{mg^2}{\pi^2} \int_0^\infty \mathcal{P} \frac{k'^2 \, n^{(0)}(k') \, dk'}{k'^2 - m^2 c_c^2} = c^2. \tag{27.15}$$

One can transform the integral on the left-hand side of (27.15) as follows

$$\int_0^\infty \mathcal{P} \frac{k'^2\, n^{(0)}(k')\, dk'}{k'^2 - m^2 c_r^2} = \int_0^\infty n^{(0)}(k')\, dk' + m^2 c_r^2 \int_0^\infty \mathcal{P} \frac{n^{(0)}(k')\, dk'}{k'^2 - m^2 c_r^2} .$$

The quantity mc_r is as a rule very small compared to characteristic electron momenta. One can thus drop the second term, and (27.15) gives at once the required sound velocity

$$c_r^2 = c^2 - \frac{m^{\frac{3}{2}} g^2}{\pi^2 \sqrt{2\beta}} F_{-\frac{1}{2}}(\beta\mu) . \qquad (27.16)$$

A direct calculation for a non-degenerate and for a completely degenerate gas shews that in the first case one makes an error of the order of βmc_r^2, and in the second case one of order $(mc_r/k_F)^2$. Both these quantities are under normal conditions completely negligible.

For a non-degenerate electron gas (27.16) becomes (in the usual units)

$$c_r^2 = c^2 - n\beta g^2 = c^2 - n\beta \frac{(E_C^{(1)})^2}{d} , \qquad (27.17)$$

The sound velocity turns thus out to be linearly dependent on the charge carrier concentration n.

We note that the quantities occurring on the right-hand sides of (27.16) and (27.17) are not positive definite for all values of the coupling constant. The quantity c_r, on the other hand, must by definition be real (if this were not the case, (27.12) would not have real roots of the form (27.13), that is, one could not propagate sound of the usual kind in the lattice). This fact imposes formally a limitation on the possible values of the coupling constant. We must, however, note that (27.16) and (27.17) were obtained in the framework of perturbation theory and it is not clear a priori whether one can apply them in a region where the corrections to c^2 are comparable to its own magnitude. To solve this problem finally one should use the renormalisation group in the same way as was done in chapter IV to determine the plasma frequencies. We shall not consider it here; we note merely that the problem of a limiting value of g^2 in a metal has been studied by different methods by a number of authors (see, for example, Fröhlich 1952, Wentzel 1952, Tolmachev and Tyablikov 1958b; in the last of these papers the adiabatic approximation was used to establish the existence of an upper limit to g^2).

One can also easily evaluate the "damping coefficient" of the phonons - assuming it to be small. Proceeding as in section 20 we get

$$\gamma = \left| \frac{(2\pi)^4 \vec{k}^2 \lim\limits_{\gamma \to +0} \operatorname{Im} \mathcal{P}^{(0)}(\vec{k}, \omega' - i\gamma)}{2\omega'(\vec{k}) - (2\pi)^4 k^2 \dfrac{\partial \operatorname{Re} \mathcal{P}^{(0)}(k)}{\partial k_0}\Big|_{k_0=\omega'}} \right| \tag{27.18}$$

We must substitute here for ω' the solution of the dispersion relation (27.12). We have, in particular, for small k, $\omega' = c_T k$. In that case the first term in the denominator dominates; using (27.11) we find

$$\gamma(\vec{k}) \cong \frac{ng^2 \sqrt{2\beta m}}{8 c_T F_{\frac{1}{2}}(\beta m)} \ln \frac{1 + e^{\beta\mu + \frac{1}{2}\beta\omega' - \frac{\beta \vec{k}^2}{2m}}}{1 + e^{\beta\mu - \frac{1}{2}\beta\omega' - \frac{\beta \vec{k}^2}{2m}}} . \tag{27.19}$$

We have dropped small terms of order $\beta m c_T^2$. As $\beta \to \infty$ ($T \to 0$), (27.19) changes to the equation obtained by Migdal (1958).

We now turn to the fermion branch of the spectrum. We have from (11.3) and (6.18) for the mass operator

$$M^{(0)}(k) = -ig^2 \int d^4k' \, G_c^{(0)}(k+k') \, D_c^{(0)}(k') . \tag{27.20}$$

We substitute here (5.20) and (27.7) and integrate over k_0' (from the rule (5.5) it follows that the contour of integration must be closed in the upper half-plane). The result is

$$\begin{aligned} M^{(0)}(k) = -\frac{g^2}{(2\pi)^7} \int d^3\vec{k}' \, \vec{k}'^2 \, \{ & n^{(0)}(\vec{k}+\vec{k}') \\ & \times \frac{[k_0 - W(\vec{k}+\vec{k}')]^2 - \omega^2(\vec{k}') - i\varepsilon [2\nu(\vec{k}') + 1]}{\{[k_0 - W(\vec{k}+\vec{k}')]^2 - \omega^2(\vec{k}')\}^2 + \varepsilon^2} \\ & - \frac{\nu(\vec{k}')}{2\omega(\vec{k}')} \cdot \frac{\omega(\vec{k}') + k_0 - W(\vec{k}+\vec{k}') + i\eta [2n^{(0)}(\vec{k}+\vec{k}') - 1]}{[\omega(\vec{k}') + k_0 - W(\vec{k}+\vec{k}')]^2 + \eta^2} \\ & - \frac{\nu(\vec{k}') + 1}{2\omega(\vec{k}')} \cdot \frac{-\omega(\vec{k}') + k_0 - W(\vec{k}+\vec{k}') + i\eta [2n^{(0)}(\vec{k}+\vec{k}') - 1]}{[-\omega(\vec{k}') + k_0 - W(\vec{k}+\vec{k}')]^2 + \eta^2} . \end{aligned} \tag{27.21}$$

We shall in the following be interested either in the real part of the mass operator for real values of k_0, or in its imaginary part for $k_0 = \omega' - i\gamma$, $\gamma \ll \omega'$. Proceeding as in section 23 we get

$$\begin{aligned} \operatorname{Re} M^{(0)}(\vec{k}, k_0 = \omega') = -\frac{g^2}{(2\pi)^7} \int d^3\vec{k}' \, \vec{k}'^2 \, \mathcal{P} & \frac{n^{(0)}(\vec{k}+\vec{k}')}{[k_0 - W(\vec{k}+\vec{k}')]^2 - \omega^2(\vec{k}')} \\ - \frac{\nu(\vec{k}')}{2\omega(\vec{k}')[\omega(\vec{k}') + k_0 - W(\vec{k}+\vec{k}')]} & - \frac{\nu(\vec{k}') + 1}{2\omega(\vec{k}')[-\omega(\vec{k}') + k_0 - W(\vec{k}+\vec{k}')]} , \end{aligned} \tag{27.22}$$

$$\lim_{\substack{\gamma\to 0\\ \gamma>0}} \operatorname{Im} M^{(0)}(\vec{k}, k_0=\omega'-i\gamma)$$

$$= \frac{g^2}{4(2\pi)^6} \int d^3\vec{k}' \frac{\vec{k}'^2}{\omega(\vec{k}')} \{[v(\vec{k}') + n^{(0)}(\vec{k}+\vec{k}')] \delta[\omega' + \omega(\vec{k}') - W(\vec{k}+\vec{k}')]$$

$$+ [v(\vec{k}') + 1 - n^{(0)}(\vec{k}+\vec{k}')] \delta[\omega' - \omega(\vec{k}') - W(\vec{k}+\vec{k}')]\} . \qquad (27.23)$$

In the Boltzmann statistics case one can easily evaluate the integral in (27.23) completely. As the region of relatively small wave numbers is the most important one we can use the approximation (27.3); it is also clear that in the important region $v(\vec{k}) \gg 1 \gg n^{(0)}(\vec{k})$ and $\omega(\vec{k}) \ll W(\vec{k})$ (the collisions are practically elastic). If we neglect quantities of the order βmc_T^2, we get then

$$\lim_{\gamma\to 0,\ \gamma>0} \operatorname{Im} M^{(0)}(\vec{k}, k_0=\omega'-i\gamma) \approx \frac{mg^2\sqrt{2m\omega'}}{(2\pi)^5 \beta c^2} \theta(\omega') . \qquad (27.24)$$

We can use (27.21) to (27.24) to study the influence of the electron-phonon interaction on different characteristic features of the system of electrons and phonons, both of equilibrium and of non-equilibrium states.

28. THE ENERGY SPECTRUM OF A SUPERCONDUCTOR *

Up to now we have performed all actual calculations within the perturbation theory framework of section 11. In the present section we shall consider a very important example where this is not possible and where the Green function as a function of the coupling constant g has an essential singularity as $g \to 0$. We consider here the problem of the energy spectrum of a superconductor in the Bardeen model, in which the electron-phonon interaction is replaced by a special form of a direct electron-electron interaction (see section 6). Using (6.5) and (6.15) we have for the Hamiltonian of this problem

$$H' = H'_p + H_{int} , \qquad (28.1)$$

$$H'_p = \Sigma_\lambda \{T(\lambda) - \mu\} a^+(\lambda) a(\lambda) , \qquad (28.2)$$

$$H_{int} = \frac{1}{2V} \sum_{\lambda,\lambda'(\lambda\neq\lambda')} B(\lambda, \lambda') a^+(\lambda) a^+(-\lambda) a(-\lambda') a(\lambda') \qquad (28.3)$$

We note that formally one can reduce the Hamiltonians of several other systems also to the same form. Apart from the specific appli-

* Bogolyubov, Tolmachev, and Shirkov 1958, Zubarev and Tserkovnikov 1959, Zubarev 1960.

cation to the theory of superconductivity, the Hamiltonian (28.1) to (28.3) is also independently of interest as it can be asymptotically diagonalised exactly (Bogolyubov, Zubarev, and Tserkovnikov 1957). In the given case λ denotes the three components of the momentum $\vec{p}$ and the spin coordinate σ ($\lambda = \{\vec{p},\sigma\}$; $-\lambda = \{-\vec{p},-\sigma\}$; $T(\lambda) = T(\vec{p}) = \vec{p}^2/2m$). The function $B(\lambda,\lambda')$ satisfies the following relations

$$B(\lambda,\lambda') = -B(\lambda,-\lambda') ; \quad B(\lambda,\lambda') = B(\lambda',\lambda) < 0 . \tag{28.4}$$

The reduction of the electron-phonon interaction to an equivalent electron-electron interaction can be effected only for electrons lying within a thin layer about the Fermi surface. It follows from this that $B(\lambda,\lambda')$ may differ appreciably from zero only in that layer. (In the Bardeen model proper one assumes that it is constant within a layer of thickness $2\omega_0$ and zero outside this layer.)

In this section we turn to the direct solution of a set of equations such as (7.7), decoupling it by means of an asymptotically exact method. We introduce the Green functions

$$G(\lambda, x_0 - x_0') = \ll a(\lambda, x_0) \mid a^+(\lambda, x_0')\gg^{(+)} , \tag{28.5}$$

$$G_2(\lambda,\lambda'; x_0 - x_0') = \ll a^+(-\lambda, x_0)a(-\lambda', x_0)a(\lambda', x_0) \mid a^+(\lambda, x_0')\gg^{(+)} . \tag{28.5'}$$

Using (28.1) to (28.3) we get from (7.7) ($x_0 - x_0' = t$, $T'(\lambda) \equiv T(\lambda) - \mu$)

$$i\frac{\partial G(\lambda,t)}{\partial t} = -\delta(t) + T'(\lambda)\, G(\lambda,t) + \frac{1}{V}\Sigma_{\lambda'} B(\lambda,\lambda')\, G_2(\lambda,\lambda;t) , \tag{28.6}$$

$$\begin{aligned} i\frac{\partial G_2(\lambda,\lambda';t)}{\partial t} &= -\delta(t)\mathfrak{n}(-\lambda)[\Delta(\lambda-\lambda') - \Delta(\lambda+\lambda')] + [2T'(\lambda') - T'(\lambda)]\, G_2(\lambda,\lambda';t) \\ &+ \frac{1}{V}\Sigma_{\lambda''} B(\lambda,\lambda'') \ll a^+(\lambda'', x_0)a^+(-\lambda'', x_0)a(-\lambda', x_0)a(\lambda', x_0)a(\lambda, x_0) \mid a^+(\lambda, x_0')\gg^{(+)} \\ &+ \frac{1}{V}\Sigma_{\lambda''} B(\lambda',\lambda'') \ll [1 - \mathfrak{n}(-\lambda') - \mathfrak{n}(\lambda')] \\ &\qquad \times a^+(-\lambda, x_0)a(-\lambda'', x_0)a(\lambda'', x_0) \mid a^+(\lambda, x_0')\gg^{(+)} \\ &+ \frac{1}{V}\Sigma_{\lambda''} B(\lambda',\lambda'')\, G_2(\lambda,\lambda'';t)\,[\Delta(\lambda+\lambda') + \Delta(\lambda-\lambda')] , \end{aligned} \tag{28.7}$$

Here, as always, Δ is the delta-function of a discrete argument (Kronecker symbol), and

$$\mathfrak{n}(\lambda) = a^+(\lambda)a(\lambda) . \tag{28.8}$$

It is of physical interest to study the asymptotic behaviour of (28.6) and (28.7) as $V \to \infty$. This makes it possible to simplify the problem appreciably. Indeed, one can shew (Zubarev 1960) that the averages of the operators $\mathfrak{n}(\lambda)$ and $V^{-1}\Sigma_{\lambda''} B(\lambda',\lambda'')a^+(-\lambda')a(-\lambda'')a(\lambda'')a^+(\lambda')$ remain finite as $V \to \infty$. We can thus assume that these operators com-

mute asymptotically and the average of their product is thus the product of their averages

$$\ll[1 - \mathfrak{n}(-\lambda') - \mathfrak{n}(\lambda')]\, a^+(-\lambda)a(-\lambda'')a(\lambda'')\,|a^+(\lambda)\gg^{(+)}$$
$$= [1 - n(\lambda') - n(-\lambda')]\; G_2(\lambda, \lambda''; t)\,. \qquad (28.9)$$

Here $n(\lambda') = <\mathfrak{n}(\lambda')> = <a^+(\lambda')a(\lambda')>$. One can transform in a similar way also the third term on the right-hand side of (28.7). It is, however, difficult to find a foundation for this method of decoupling. This justification follows from the results of a paper by Bogolyubov, Zubarev, and Tserkovnikov (1960) who shewed that it allows us to solve the whole chain of Green function equations asymptotically exactly. Bogolyubov (1960) has given a mathematical proof of the fact that the solution obtained in this way differs from the exact one by terms of the order $1/N$.

Moreover, the term G_2 occurs in (28.6) with a factor $1/V$; we can thus in (28.7) asymptotically neglect terms containing $\Delta(\lambda \pm \lambda')$.

The second simplification is, as the first one, connected in the final reckoning with the form of the pair term (28.3) in the Hamiltonian (28.1); we sum there over only two (and not over four) variables.

The equations of motion are thus

$$i\,\frac{\partial G(\lambda, t)}{\partial t} = -\,\delta(t) + T'(\lambda)G(\lambda, t) + \frac{1}{V}\,\Sigma_{\lambda'}\, B(\lambda, \lambda')G_2(\lambda, \lambda'; t)\,; \qquad (28.10)$$

$$i\,\frac{\partial G_2(\lambda, \lambda'; t)}{\partial t} = [2T'(\lambda') - T'(\lambda)]\; G_2(\lambda, \lambda'; t)$$
$$+ \frac{1}{V}\,\Sigma_{\lambda''}\, B(\lambda, \lambda'')\, <a^+(\lambda'')a^+(-\lambda'')a(-\lambda')a(\lambda')>\; G(\lambda, t)$$
$$+ \frac{1}{V}\,\Sigma_{\lambda''}\, B(\lambda', \lambda'')\,[1 - n(-\lambda') - n(\lambda')]\; G_2(\lambda, \lambda''; t)\,. \qquad (28.11)$$

All four operators under the averaging sign in the second term on the right-hand side of (28.11) are taken at the same time - immaterial which time, as the average is independent of the time. We introduce, as usual, the Fourier transform of the Green functions, putting

$$G(\lambda, t) = \int_{-\infty}^{+\infty} dE\; G(\lambda, E)\; e^{-iEt}\,,$$

$$G_2(\lambda, \lambda'; t) = \int_{-\infty}^{+\infty} dE\; G_2(\lambda, \lambda'; E)\; e^{-iEt}\,. \qquad (28.12)$$

We get

$$E\,G(\lambda,E) = -\frac{1}{2\pi} + T'(\lambda)G(\lambda,E) + \frac{1}{V}\Sigma_{\lambda'}\,B(\lambda,\lambda')\,G_2(\lambda,\lambda';E)\,, \qquad (28.13)$$

$$E\,G_2(\lambda,\lambda';E) = [2T'(\lambda') - T'(\lambda)]\,G_2(\lambda,\lambda';E)$$
$$+\frac{1}{V}\Sigma_{\lambda''}\,B(\lambda,\lambda'')\,\langle a^+(\lambda'')a^+(-\lambda'')a(-\lambda')a(\lambda')\rangle\,G(\lambda,E)$$
$$+\frac{1}{V}\Sigma_{\lambda''}\,B(\lambda',\lambda'')\,[1-n(\lambda')-n(-\lambda')]\,G_2(\lambda,\lambda'';E)\,. \qquad (28.14)$$

This set of equations we shall solve exactly.

We put

$$\langle a^+(\lambda'')a^+(-\lambda'')a(-\lambda')a(\lambda')\rangle = f(\lambda'')\,f(\lambda')\,, \qquad (28.15)$$

$$G_2(\lambda,\lambda';E) = \varphi(\lambda,E)\,f(\lambda')\,, \qquad (28.16)$$

where f and φ are new unknown functions and $f(\lambda) = f^+(\lambda)$. Substituting these expressions into (28.13) and (28.14) we find

$$[E - T'(\lambda)]\,G(\lambda,E) = -\frac{1}{2\pi} + \frac{1}{V}\Sigma_{\lambda'}\,B(\lambda,\lambda')\,\varphi(\lambda,E)\,f(\lambda')\,,$$

$$[E + T'(\lambda)]\,\varphi(\lambda,E)\,f(\lambda') = \frac{1}{V}\Sigma_{\lambda''}\,B(\lambda,\lambda'')\,f(\lambda'')\,g(\lambda,E)\,f(\lambda')$$
$$+ 2T'(\lambda')\,\varphi(\lambda,E)\,f(\lambda')$$
$$+\frac{1}{V}\Sigma_{\lambda''}\,B(\lambda',\lambda'')\,f(\lambda'')\,[1 - n(\lambda') - n(-\lambda')]\,\varphi(\lambda,E)\,. \qquad (28.17)$$

We introduce the notation

$$\frac{1}{V}\Sigma_{\lambda''}\,B(\lambda,\lambda'')\,f(\lambda'') = L(\lambda)\,, \qquad (28.18)$$

and impose on $f(\lambda')$ the condition

$$2T'(\lambda') + \frac{L(\lambda')}{f(\lambda')}[1 - n(\lambda') - n(-\lambda')] = 0\,. \qquad (28.19)$$

The set (28.17) then simplifies to

$$\begin{aligned}[E - T'(\lambda)]\,G(\lambda,E) - L(\lambda)\,\varphi(\lambda,E) &= -\frac{1}{2\pi}\,,\\ [E + T'(\lambda)]\,\varphi(\lambda,E) - L(\lambda)\,G(\lambda,E) &= 0\,.\end{aligned} \qquad (28.20)$$

Hence

$$G(\lambda,E) = -\frac{1}{2\pi}\cdot\frac{E + T'(\lambda)}{E^2 - T'^2(\lambda) - L^2(\lambda)}\,, \qquad (28.21)$$

$$\varphi(\lambda,E) = -\frac{1}{2\pi}\cdot\frac{L(\lambda)}{E^2 - T'^2(\lambda) - L^2(\lambda)} \qquad (28.22)$$

The poles of $G(\lambda,E)$ determine the energy spectrum of the system

$$\omega(\lambda) = \sqrt{T'^2(\lambda) + L^2(\lambda)} \,. \tag{28.23}$$

One can also easily find the spectral function for the product of fermion operators and the average energy of the system. If we wrtte

$$\langle a^+(\lambda, x_0') a(\lambda, x_0) \rangle = \int_{-\infty}^{+\infty} dE\, J(\lambda, E)\, e^{-iE(x_0 - x_0')}\, e^{-\beta E} \,, \tag{28.24}$$

we get from (2.7), (3.11), (28.21), and (28.23)

$$J(\lambda, E)\, e^{-\beta E} = \tfrac{1}{2}\left[1 + \frac{T'(\lambda)}{\omega(\lambda)}\right] \frac{\delta[E - \omega(\lambda)]}{1 + e^{\beta\omega(\lambda)}} + \tfrac{1}{2}\left[1 - \frac{T'(\lambda)}{\omega(\lambda)}\right] \frac{\delta[E + \omega(\lambda)]}{1 + e^{-\beta\omega(\lambda)}} \,. \tag{28.25}$$

In the approximation used here the spectral function has thus a delta-function form and there is no damping. This is a characteristic feature of the model Hamiltonian (28.1) - which, strictly speaking, makes it possible to diagonalise it exactly.

Equations (28.21) to (28.25) are not yet the final answer as they contain the unknown function $L(\lambda)$. To determine this function we use (28.18) expressing $f(\lambda)$ in terms of $L(\lambda)$ through (28.19). Putting $x_0 = x_0'$ in (28.24) and using (28.25) we get

$$n(\lambda) = \int_{-\infty}^{+\infty} (\lambda, E)\, e^{-\beta E}\, dE = \tfrac{1}{2}\left[1 - \frac{T'(\lambda)}{\omega(\lambda)} \tanh \tfrac{1}{2}\beta\omega(\lambda)\right] . \tag{28.26}$$

From (28.26) and (28.29) we get

$$f(\lambda) = -\frac{L(\lambda)}{2\omega(\lambda)} \tanh \tfrac{1}{2}\beta\omega(\lambda) \,; \tag{28.27}$$

substituting this into (28.18) we find the following equation for $L(\lambda)$

$$L(\lambda) = -\frac{1}{2V} \Sigma_{\lambda'} B(\lambda, \lambda') \frac{L(\lambda')}{\omega(\lambda')} \tanh \tfrac{1}{2}\beta\omega(\lambda') \,. \tag{28.28}$$

If we determine from this equation $L(\lambda)$ we find both the energy spectrum (28.23) and the average energy of the system. Indeed, from (28.1), (28.15), (28.18), and (28.27) we have

$$\langle H' \rangle = \Sigma_\lambda\, T'(\lambda)\, n(\lambda) + \frac{1}{2V} \sum_{\lambda, \lambda'} B(\lambda, \lambda')\, f(\lambda)\, f(\lambda')$$

$$= \tfrac{1}{2} \sum_{\lambda} \left\{ T'(\lambda) \left[1 - \frac{T'(\lambda)}{\omega(\lambda)} \tanh \frac{\beta\omega(\lambda)}{2}\right] - \frac{L^2(\lambda)}{2\omega(\lambda)} \tanh \frac{\beta\omega(\lambda)}{2} \right\} . \tag{28.29}$$

In particular, we get from (28.29) the ground state energy of the system as $\beta \to \infty$.

Let us now solve (28.28) following Zubarev and Tserkovnikov (1959). We change the summation over $\vec{k}$ to an integration and introduce a new variable

$$\xi = T'(\lambda) \,. \tag{28.30}$$

It is clear from the symmetry of the problem that $L(\lambda)$ in fact depends on ξ only; equation (28.28) becomes thus

$$L(\xi) = -\frac{1}{(2\pi)^2}\int_0^{\omega_0} k'^2(\xi')\frac{dk'}{d\xi'}d\xi' \tanh\tfrac{1}{2}\beta\omega(\xi')\frac{L(\xi')}{2\omega(\xi')}\int_{-1}^{+1} B(\xi,\xi';l)\,dl\,, \tag{28.31}$$

where l is the cosine of the angle between $\vec{k}$ and $\vec{k}'$. The integral of $B(\xi,\xi';l)$ over l plays in (28.31) the role of the kernel. For the following it is convenient to normalise the kernel in such a way that it becomes equal to unity as $\xi = \xi' = 0$. We put thus

$$\tfrac{1}{2}\int_{-1}^{+1} dl\; B(\xi,\xi';l) = B\,F\left(\frac{\xi}{\omega_0},\frac{\xi'}{\omega_0}\right), \tag{28.32}$$

where F is a dimensionless function and

$$B = \tfrac{1}{2}\int_{-1}^{+1} dl\; B(0,0;l) < 0\,. \tag{28.33}$$

It is clear that

$$F(0,0) = 1\,. \tag{38.34}$$

We also introduce a new unknown function $\chi(\xi)$ putting

$$L(\xi) = C\,\chi(\xi)\,, \qquad \chi(0) = 1 \qquad (C = \text{constant})\,. \tag{28.35}$$

Because the region of integration over ξ in (28.31) is a narrow one, one can take the Jacobian $k'^2\,(dk'/d\xi')$ from under the integral sign putting it equal to its value at $k = k_F$; we get thus in front of the integral the factor

$$\rho = \frac{|B|}{(2\pi)^2}\left(k^2\frac{dk}{d\xi}\right)_{k=k_F}. \tag{28.36}$$

Finally, it is convenient to introduce dimensionless quantities by putting

$$x = \frac{\xi}{\omega_0}\,, \quad \epsilon(x) = \frac{\omega(\xi)}{\omega_0} = \sqrt{x^2 + b^2\,\chi^2(x)}\,, \quad b = \frac{C}{\omega_0}\,, \quad a = \frac{2}{\beta\omega_0}\,. \tag{28.37}$$

We get then from (28.31)

$$\chi(x) = \rho\int_0^{\infty} dx'\,F(x,x')\frac{\chi(x')}{\epsilon(x')}\tanh\frac{\epsilon(x')}{a}\,. \tag{28.38}$$

Assuming that the electron-phonon interaction is rather weak and that the temperature is low, we may assume that a and b are small quantities. It turns, however, out to be impossible to expand $\chi(x)$ directly into a power series in b as (28.38) has a logarithmic singularity at $x = 0$ as $b \to 0$, $a \to 0$, a/b = constant. This was the reason also why we could not apply standard perturbation theory to the present problem.

To get rid of this singularity we put $x = 0$ in (28.38), multiply the expression obtained in this way by $F(x,0)$ and evaluate the result termwise from (28.38). Using (28.35) we get

$$\chi(x) = F(x,0) + \rho \int_0^\infty dx' \{F(x,x') - F(x,0)\, F(0,x')\} \frac{\chi(x')}{\epsilon(x')} \tanh \frac{\epsilon(x')}{a}. \tag{28.39}$$

The expression within the braces vanishes for $x = 0$ because of (28.34) and this makes it possible to take the limit $a \to 0$, $b \to 0$. We get then a non-singular linear equation

$$\chi(x) = F(x,0) + \rho \int_0^\infty dx' \frac{F(x,x') - F(x,0)F(0,x')}{x'} \chi(x'), \tag{28.40}$$

which can be solved by the usual methods. In particular, we have in the Bardeen model $F(x,x') = 1$ for $0 \le x \le 1$, $0 \le x' \le 1$, and $F(x,x') = 0$ otherwise; we get thus $\chi(x) = F(x,0)$, and hence

$$\epsilon(x) = \sqrt{x^2 + b^2} = \sqrt{x^2 + C^2/\omega_0^2};$$

substituting this expression into (28.38) we get an equation to determine C and thus L:

$$1 = \rho \int_0^1 dx \frac{\tanh \dfrac{\sqrt{x^2 + C^2\,\omega_0^{-2}}}{a}}{\sqrt{x^2 + C^2\,\omega_0^{-2}}}. \tag{28.41}$$

It follows from (28.23) and (28.35) that as $C \neq 0$ the elementary excitation spectrum does not begin at zero for the system considered, but it starts from a finite value, which is equal to $|C|$ (the gap). This is in final reckoning responsible for the superconductivity (Bogolyubov, Tolmachev, and Shirkov 1958). Bogolyubov, Zubarev, and Tserkovnikov (1957) and Zubarev and Tserkovnikov (1959) have shewn from a study of (28.41) that there is in fact a gap only provided a is sufficiently small, and that this determines the critical temperature for the transition into the superconducting state. We restrict ourselves to just evaluating the spectrum at absolute zero ($\beta \to \infty$). We get then from (28.41)

$$C = 2\omega_0\, e^{-1/\rho}, \tag{28.42}$$

and thus

$$\omega(\vec{k}) = \sqrt{T'^2(\vec{k}) + 4\omega_0^2\, e^{-2/\rho}}. \tag{28.43}$$

We see now from (28.36) that the energy $\omega(\vec{k})$ considered as a function of the "interaction parameter" B has an essential singularity as $B \to 0$. This is a consequence of the singularity of (28.38), that is, in final reckoning a consequence of the peculiar features of the system which are reflected in the special structure of the Hamiltonian (28.1).

Chapter VII

FERROMAGNETISM

29. SPIN WAVES AT FINITE TEMPERATURES *

In this chapter we shall apply the Green function method to study a very simple problem in ferromagnetism: the problem of evaluating the magnetisation of an isotropic ferromagnet as function of the temperature and the external field. We must note that there are well-proven and effective methods for calculating this both at low and at high temperatures. For low temperatures ($T \ll T_c$, T_c: Curie temperature) we have the spin-wave and approximate-second-quantisation methods (the basic ideas of the latter are given by Bogolyubov and Tyablikov, 1957) which derive from Bloch's well-known paper (1929). In this region Dyson (1956a,b) made some important progress. He obtained a series expansion in powers of the temperature which enabled him to extend the region of applicability of the spin wave formalism up to temperatures of the order of $T_c/4$. These results have recently been obtained also by other methods (Opechowski 1959). When the temperature becomes higher the situation gets somewhat worse, and for $T \sim T_c$ there is essentially only the very rough molecular field method (see, for instance, Vonsovskiĭ and Shur 1048). Finally, if $T \gg T_c$ one can use the usual perturbation theory methods. In that case one gets an expansion of the magnetisation in inverse powers of the temperature (Opechowski 1937).

There are thus in the theory of ferromagnetism different methods for evaluating the free energy, the magnetisation, and so on, each of which is valid only in its own temperature range. We shall see that it turns out to be possible by using Green function methods to develop one approximate method which is valid in the whole temperature range to evaluate the magnetisation(Tyablikov 1959).

Let the ferromagnet studied here consist of N atoms of a ferromagnetic element which form a regular, simple lattice. We shall, moreover, assume that each atom has only a single "ferromagnetic" electron and that we may neglect the interaction between these electrons and the conduction electrons. Finally, we shall take into account only the exchange interaction between the electrons and assume that magnetically speaking our ferromagnetic is isotropic. Under these circumstances the system considered is described by a Heisen-

* Bogolyubov and Tyablikov 1959, Tyablikov 1959.

berg Hamiltonian which can be expressed in terms of Pauli operators (see (6.19)):

$$H = C + [2\mu_B\mathcal{H} + 2A'(0)] \sum_{\vec{f}} \mathfrak{n}(\vec{f}) - 2 \sum_{\vec{f}_1,\vec{f}_2} A(\vec{f}_1 - \vec{f}_2) b^+(\vec{f}_1) b(\vec{f}_2)$$

$$\sum_{\vec{f}_1,\vec{f}_2} 2A(\vec{f}_1 - \vec{f}_2)\, \mathfrak{n}(\vec{f}_1)\, \mathfrak{n}(\vec{f}_2) \,. \tag{29.1}$$

Here

$$C = -\tfrac{1}{2} NA'(0) - N\mu_B\mathcal{H} \,, \qquad \mathfrak{n}(\vec{f}) = b^+(\vec{f}) b(\vec{f}) \,,$$

$$A'(\vec{k}) = \sum_{\vec{f}} A(\vec{f})\, e^{i(\vec{k}\cdot\vec{f})} \,; \qquad A(0) = 0 \,; \tag{29.2}$$

$\vec{f}$ enumerates the lattice sites, $A(\vec{f}_1 - \vec{f}_2)$ is the exchange integral for electrons on the sites $\vec{f}_1$ and $\vec{f}_2$, $A'(\vec{k})$ the Fourier transform of $A(\vec{f})$, $\mathcal{H}$ the magnitude of the external magnetic field, and μ_B the Bohr magneton.

Following the method described in section 6 we introduce the Green functions

$$G(\vec{g},\vec{f}\,; x_0 - x_0') = \ll b(\vec{g}, x_0) \,|\, b^+(\vec{f}, x_0') \gg^{(-)} \,, \tag{29.3}$$

$$G_2(\vec{g}_1, \vec{g}_2, \vec{f}\,; x_0 - x_0') = \ll \mathfrak{n}(\vec{g}_1, x_0) b(\vec{g}_2, x_0) \,|\, b^+(\vec{f}, x_0') \gg^{(-)} \,, \tag{29.3a}$$

and write down their equations of motion. Using (29.1) for the Hamiltonian and the commutation relations for the Pauli operators, and putting $x_0 - x_0'$ we find easily

$$i\frac{\partial G(\vec{g},\vec{f}\,;t)}{\partial t} = -(1-2n)\,\Delta(\vec{g}-\vec{f})\,\delta(t) + [2\mu_B\mathcal{H} + 2A'(0)]\, G(\vec{g},\vec{f}\,;t)$$

$$- \sum_{\vec{g}'} 2A(\vec{g}-\vec{g}')\, G(\vec{g}', \vec{f}\,; t)$$

$$+ \sum_{\vec{g}'} 4A(\vec{g}-\vec{g}') \,[G_2(\vec{g},\vec{g}',\vec{f}\,;t) - G_2(\vec{g}',\vec{g},\vec{f}\,;t)] \,; \ldots \tag{29.4}$$

Here n is the average of the operator $b^+(\vec{g})b(\vec{g})$:

$$n = \langle b^+(\vec{g}) b(\vec{g}) \rangle \,. \tag{29.5}$$

which is independent of $\vec{g}$. We can in the same way also easily find the equations of motion for $G_2(\vec{g}_1,\vec{g}_2,\vec{f}\,;t)$, and so on. We shall not write down here the next equation as we shall restrict our considerations to the first Green function only.

We shall decouple the chain of equations (29.4) at the first equation, by putting

$$G_2(\vec{g}_1,\vec{g}_2,\vec{f};t) = \ll \mathfrak{N}(\vec{g}_1,x_0)b(\vec{g}_2,x_0)\,|\,b^+(\vec{f},x_0')\gg^{(-)}$$

$$\cong \langle \mathfrak{N}(\vec{g}_1)\rangle \ll b(\vec{g}_2,x_0)\,|\,b^+(\vec{f},x_0')\gg^{(-)}$$

$$= nG(\vec{g}_2,\vec{f};t)\,. \qquad (29.6)$$

Substituting this expression into (29.4) we get the following first approximation equation

$$i\frac{\partial G(\vec{g},\vec{f};t)}{\partial t} - [2\mu_B\mathcal{H} + (1-2n)\,2A'(0)]\,G(\vec{g},\vec{f};t) + \sum_{\vec{g}'}(1-2n)\,2A(\vec{g}-\vec{g}')\,G(\vec{g}',\vec{f};t) = -(1-2n)\,\Delta(\vec{g}-\vec{f})\,\delta(t)\,. \qquad (29.7)$$

We note that the proposed method of decoupling in first approximation as applied to ferromagnetism corresponds to the method of approximation as applied to ferromagnetism corresponds to the method of approximate second quantisation (Bogolyubov and Tyablikov 1949a). Indeed, in that method – when applied to ferromagnetism – the Pauli operators $b(\vec{f})$ and $b^+(\vec{f})$ are (approximately) considered to be boson operators and the last term in (29.1) is dropped. If we then write down the equations for the Green functions they are the same as (29.7) with $n = 0$. The chain of equations is then reduced to the first one. One can improve this method by taking out of the dropped term a part involving $n\,\mathfrak{N}(\vec{g})$ and taking that into account; one can then obtain an equation such as (29.7).

We now change from $G(\vec{g},\vec{f};t)$ to its Fourier transform

$$G(\vec{g},\vec{f};t) = \int_{-\infty}^{+\infty} G(\vec{g},\vec{f};E)\,e^{-iEt}\,dE\,. \qquad (29.8)$$

We then get from (29.7)

$$\{E - 2\mu_B\mathcal{H} - (1-2n)\,2A'(0)\}\,G(\vec{g},\vec{f};E) + \sum_{\vec{g}'}(1-2n)\,2A(\vec{g}-\vec{g}')\,G(\vec{g}',\vec{f};E) = -\frac{1}{2\pi}(1-2n)\,\Delta(\vec{g}-\vec{f})\,. \qquad (29.9)$$

Furthermore, putting

$$G(\vec{g},\vec{f};E) = \frac{1}{N}\sum_{\vec{k}} e^{-i(\vec{g}-\vec{f}\cdot\vec{k})}\,G(\vec{k},E)\,, \qquad (29.10)$$

we get (compare (5.15) and (5.16))

$$G(\vec{k},E) = -\frac{1}{2\pi}\cdot\frac{1-2n}{E - W(\vec{k})}\,, \qquad (29.11)$$

where

$$W(\vec{k}) = 2\mu_B\mathcal{H} + (1-2n)\,[2A'(0) - 2A'(\vec{k})]\,. \qquad (29.12)$$

From (29.12) and (4.6) we get the following expression for the spectral function

$$J(\vec{k}, E) = \frac{1 - 2n}{1 - e^{-\beta W(\vec{k})}} \delta[E - W(\vec{k})] , \tag{29.13}$$

and thus, from (29.10),

$$J(\vec{g}, \vec{f}; E) = \frac{1}{N} \sum_{\vec{k}} \frac{1 - 2n}{1 - e^{-\beta W(\vec{k})}} \delta[E - W(\vec{k})] \, e^{i(\vec{g}-\vec{f}\cdot\vec{k})} . \tag{29.14}$$

We can now use (2.7) which expresses the average of a product of operators in terms of the appropriate spectral function:

$$\begin{aligned} \langle b^+(\vec{f}, x_0') b(\vec{g}, x_0) \rangle &= \int_{-\infty}^{+\infty} e^{-iE(x_0 - x_0')} J(\vec{g}, \vec{f}; E) \, e^{-\beta E} \, dE \\ &= \frac{1}{N} \sum_{\vec{k}} e^{i(\vec{g}-\vec{f}\cdot\vec{k}) - iW(\vec{k})(x_0 - x_0')} \frac{1 - 2n}{e^{\beta W(\vec{k})} - 1} \end{aligned} \tag{29.15}$$

If we now put $x_0 = x_0'$ and $\vec{g} = \vec{f}$, we get an equation from which we can determine the quantity n from (29.5) which has so far not yet been determined:

$$n = \frac{1 - 2n}{N} \sum_{\vec{k}} \frac{1}{e^{\beta W(\vec{k})} - 1} , \tag{29.16}$$

or, if we change the summation over $\vec{k}$ to an integration

$$n = (1 - 2n) \frac{v}{(2\pi)^3} \int \frac{d^3\vec{k}}{e^{\beta W(\vec{k})} - 1} , \tag{29.17}$$

where $v = V/N$ is the elementary cell volume while the integral over $\vec{k}$ is over a cell of the reciprocal lattice.

For the sake of convenience we introduce the relative magnetisation σ defined as the magnetisation per site. Noting that the z-component of the spin is connected with the spin-deviation operator $\mathfrak{n} = b^+b$ by (II.3) we can write

$$\sigma \equiv \langle \sigma_z(\vec{g}) \rangle = \langle 1 - 2\mathfrak{n}(\vec{g}) \rangle = 1 - 2n . \tag{29.18}$$

We get then from (29.17) the relation

$$\frac{1}{\sigma} = \frac{v}{(2\pi)^3} \int \coth \tfrac{1}{2} \beta W(\vec{k}) \, d^3\vec{k} . \tag{29.19}$$

We see from (29.11) that the Green function Fourier transform $G(\vec{k}, E)$ has a pole at $E = W(\vec{k})$ and $W(\vec{k})$ is thus the energy of an elementary excitation in a ferromagnetic: the "spin-wave" energy. The expression for $W(\vec{k})$ is of the same form as the usual formula for the spin-wave energy

$$W_{\text{sp.w.}}(\vec{k}) = 2\mu_B\mathcal{H} + 2A'(0) - 2A(\vec{k}) , \qquad (29.20)$$

which differs from $W(\vec{k})$ by the terms involving the wave vector which in $W(\vec{k})$ are proportional to the relative magnetisation $\sigma = 1 - 2n$, given by (29.18). Because of this factor the elementary excitation energy $W(\vec{k})$ depends on the temperature.

30. THE MAGNETISATION IN DIFFERENT TEMPERATURE RANGES *

In our first approximation we have reduced the problem of determining the relative magnetisation as a function of temperature and external field to solving (29.19). We shall now shew that this equation gives a rather satisfactory interpolation for the magnetisation for all temperatures. To do this we shall prove that we get for $T \ll T_c$ Bloch's well-known result (1929) for σ, for $T \lesssim T_c$ the result of the molecular field approximation, and for $T \gg T_c$ the results of the theory of paramagnetism.

For the sake of convenience we introduce dimensionless quantities

$$L = \frac{\mu_B\mathcal{H}}{A'(0)} , \qquad \tau = \frac{1}{\beta A'(0)} , \qquad \epsilon(\vec{k}) = 1 - \frac{A'(\vec{k})}{A'(0)} , \qquad (30.1)$$

(the constant $A'(0) = \Sigma_{\vec{f}} A(\vec{f})$ is the average value of the exchange interaction and is proportional to the Curie temperature: compare (30.14) and the definition of τ), and we write (29.19) in dimensionless form

$$\frac{1}{\sigma} = \frac{v}{(2\pi)^3} \int \coth \frac{L + \sigma\epsilon(\vec{k})}{\tau} \, d^3\vec{k} . \qquad (30.2)$$

Let us first consider the low-temperature case. We have then $\tau \to 0$, $L + \sigma\epsilon(\vec{k}) \gg \tau$ and we can use the expansion

$$\coth \xi = 1 + 2 \sum_{l=1}^{\infty} e^{-2l\xi} .$$

We can then write (30.2) in the form

$$\frac{1}{\sigma} = 1 + \mathcal{P}(\frac{\tau}{\sigma}; \frac{L}{\tau}) ; \qquad \mathcal{P} = \sum_{l=1}^{\infty} \frac{v}{(2\pi)^3} \int \exp\left(-2l \frac{L + \sigma\epsilon(\vec{k})}{\tau}\right) d^3\vec{k} . \qquad (30.3)$$

From this equation we can easily find the main term in the expansion of σ in powers of the dimensionless temperature τ. We need only bear in mind that the main contribution to the integral in (30.3) comes from the small wavevector region so that we may approximately write

$$\epsilon(\vec{k}) \cong \gamma\vec{k}^2 , \qquad \gamma = \frac{1}{\delta A'(0)} \sum_{\vec{f}} \vec{f}^2 A(\vec{f}) . \qquad (30.4)$$

* Tyablikov 1959.

We get then for $\mathcal{P}$

$$\mathcal{P}(\frac{\tau}{\sigma};\frac{L}{\tau}) = 2v\,(\frac{\tau}{8\pi\gamma\sigma})^{\frac{3}{2}}\, z_{\frac{3}{2}}(\frac{L}{\tau})\ , \tag{30.5}$$

where

$$z_p(x) = \sum_{l=1}^{\infty} l^{-p}\, e^{-lx}\ . \tag{30.6}$$

We can thus write (30.3) in the form

$$\sigma = 1 - 2v\,(\frac{\tau}{8\pi\gamma\sigma})^{\frac{3}{2}}\, z_{\frac{3}{2}}(\frac{L}{\tau})\,\sigma\ . \tag{30.7}$$

We shall solve this equation by iteration and put as zeroth approximation $\sigma_0 = 1$. We get then up to terms of order $\tau^{\frac{3}{2}}$

$$\sigma \cong 1 - 2v\,(\frac{\tau}{8\pi\gamma})^{\frac{3}{2}}\, z_{\frac{3}{2}}(\frac{L}{\tau})\ , \tag{30.8}$$

which is the same as the result of Bloch's spin-wave method. To obtain an expression for σ in a power series in τ we expand $\epsilon(\vec{k})$ in powers of k and evaluate $\mathcal{P}$ as a function of the ratio τ/σ:

$$\mathcal{P}(\frac{\tau}{\sigma};\frac{L}{\tau}) = a_1(\frac{L}{\tau})\,(\frac{\tau}{\sigma})^{\frac{3}{2}} + a_2(\frac{L}{\tau})\,(\frac{\tau}{\sigma})^{\frac{5}{2}} + a_3(\frac{L}{\tau})\,(\frac{\tau}{\sigma})^{\frac{7}{2}} + \ldots \tag{30.9}$$

Here a_1, a_2, a_3, ... are functions of L/τ. If we then solve (30.3) for σ we get

$$\sigma = 1 - \sum_{j\geq 3} A_j\, \tau^{j/2}\ , \tag{30.10}$$

where A_j are functions of L/τ which depend also on the lattice structure. In particular,

$$A_3 = \frac{2v}{(8\pi\gamma)^{\frac{3}{2}}}\, z_{\frac{3}{2}}(\frac{L}{\tau})\ , \qquad A_4 = 0\ . \tag{30.11}$$

Let us as an example consider a simple cubic lattice and take into account only nearest-neighbour interactions. For the first few coefficients A_j we get

$$A_3 = 2\,(\frac{3}{4\pi})^{\frac{3}{2}}\, z_{\frac{3}{2}}\ , \qquad A_4 = 0\ , \qquad A_5 = \frac{3\pi}{2}\,(\frac{3}{4\pi})^{\frac{5}{2}}\, z_{\frac{5}{2}}\ ,$$

$$A_6 = 2\,(\frac{3}{4\pi})^{3}\, z_3\ , \qquad A_7 = \frac{33\pi^2}{16}\,(\frac{3}{4\pi})^{\frac{7}{2}}\, z_{\frac{7}{2}}\ , \tag{30.12}$$

$$A_8 = 6\pi\,(\frac{3}{4\pi})^{4}\, z_{\frac{3}{2}}\, z_{\frac{5}{2}}, \ldots$$

We see from (30.10) to (30.12) that for the low-temperature case the first two terms in the expansion for the relative magnetisation give Bloch's results, while the later terms give corrections to them.

It is of interest to compare (30. 10) to (30. 12) with Dyson's results (1956a, b) who found for the expansion (30. 10) $A_4 = A_6 = 0$, and for the simple cubic lattice $A_8 = 10\pi\,(3/4\pi)^4\, z_{\frac{3}{2}} z_{\frac{5}{2}}$ (in our notation). One may think that the discrepancy between our results and those of Dyson's are connected with the decoupling procedure *.

We turn now to the case of high temperatures and no external field ($T \lesssim T_c$, $L = 0$). We note first of all that the system considered here has a phase transition point above which the spontaneous magnetisation vanishes. Indeed, as $\tau \to \infty$ the quantity $\sigma \leq 1$, and thus $\sigma\epsilon(\vec{k})/\tau \to 0$. Since $\coth \zeta \to 1/\zeta$ as $\zeta \to 0$, we get from (30. 2)

$$\frac{1}{\sigma} \approx \frac{\tau}{\sigma} \cdot \frac{v}{(2\pi)^3} \int \frac{d^3\vec{k}}{\epsilon(\vec{k})} . \tag{30.13}$$

From this it follows that there is no solution if the temperature is sufficiently high. To study the temperature dependence of the solution we shall, as usual, assume that $\sigma \to 0$ as $\tau \to \tau_c$ ($\tau < \tau_c$). We shall call the constant τ_c the Curie temperature. For small ζ ($\zeta = \sigma\epsilon(\vec{k})/\tau$) we have

$$\coth \zeta = \frac{1}{\zeta} + \sum_{l=1}^{\infty} 2^{2l} \frac{2l}{(2l)!}\, \zeta^{2l-1} ,$$

where B_{2l} are the Bernouilli numbers ($B_2 = \frac{1}{6}$, $B_4 = -\frac{1}{30}$, ...). Substituting this expansion into (30. 2) and introducing the notation

$$\frac{1}{\tau_c} = \frac{v}{(2\pi)^3} \int \frac{d^3\vec{k}}{\epsilon(\vec{k})} , \tag{30.14}$$

we get

$$\frac{1}{\sigma} = \frac{\tau}{\tau_c} \cdot \frac{1}{\sigma} + \sum_{l=1}^{\infty} \frac{2^{2l}\, B_{2l}}{(2l)!} \left(\frac{\sigma}{\tau}\right)^{2l-1} C_{2l-1} , \tag{30.15}$$

where

$$C_n = \frac{v}{(2\pi)^3} \int \epsilon^n(\vec{k})\, d^3\vec{k} \tag{30.15a}$$

(clearly $C_1 = 1$). We get thus

$$\frac{\sigma}{\tau} = \sqrt{\frac{3}{\tau}\left(1 - \frac{\tau}{\tau_c}\right)} \left\{1 + 3 \sum_{l=2}^{\infty} \frac{2^{2l}\, B_{2l}}{(2l)!}\, C_{2l-1} \left(\frac{\sigma}{\tau}\right)^{2l-2}\right\}^{-\frac{1}{2}} . \tag{30.16}$$

It is convenient to use an iteration method to solve this equation. In particular, we have in zeroth approximation

$$\sigma \approx \tau \sqrt{\frac{3}{\tau}\left(1 - \frac{\tau}{\tau_c}\right)} , \tag{30.17}$$

which corresponds to the usual molecular field approximation.

* (Note by translator) For a discussion of this point we may refer to recent investigations by Tahir-Kheli (1962; see also appendix VII).

It is clear both from (30.17) and from (30.16) that there is a solution only if $\tau < \tau_c$, and that this solution vanishes at $\tau = \tau_c$. The quantity τ_c defined by (30.14) is the Curie temperature.

In the nearest-neighbour approximation we can take as the unit of energy $A'(0) = \nu A$ (A: magnitude of the exchange integral and ν the number of nearest neighbours). One can then easily find the numerical value of the Curie temperature. We get for the three cubic lattices (simple cubic, body-centred cubic, and face-centred cubic) respectively

$$\tau_c = 0.66 \text{ (s.c.)}; \; 0.725 \text{ (b. c. c.)}; \; 0.745 \text{ (f. c. c.)}. \tag{30.18}$$

For temperatures near τ_c one can find a power series expansion for σ in powers of the square root of the difference $\tau_c - \tau$. We give here, as before, the first few terms of the series for a simple cubic lattice in the nearest-neighbour approximation

$$\sigma = \tau u \{1 + 5 \cdot 10^{-2} u^2 - 5 \cdot 10^{-4} u^4 + \ldots\}, \qquad u = \sqrt{\frac{3}{\tau}\left(1 - \frac{\tau}{\tau_c}\right)}. \tag{30.19}$$

We consider, finally, the temperature region above the Curie point for the case where there is a field present ($\tau \gtrsim \tau_c$; $L \neq 0$).

It is desirable to get here a solution in such a form that we can compare it with Opechowski's results (1937). To do this we write (30.2) in the form

$$\frac{1}{\sigma} = \frac{1}{t_0}\left\{1 + (1 - t_0^2) \sum_{l=1}^{\infty} \frac{(-1)^l}{t_0^l} \frac{v}{(2\pi)^3} \int [\tanh \frac{\sigma \varepsilon(\vec{k})}{\tau}]^l \, d^3\vec{k}\right\}, \qquad t_0 = \tanh \frac{L}{\tau}. \tag{30.20}$$

If we use the expansion of the hyperbolic tangent in powers of its argument and restrict ourselves to terms up to $(\sigma/\tau)^2$ we get the following approximate equation for σ:

$$\frac{1}{\sigma} = \frac{1}{t_0}\left\{1 - \frac{1 - t_0^2}{t_0} \frac{\sigma}{\tau} + \frac{1 - t_0^2}{t_0^2} \left(\frac{\sigma}{\tau}\right)^2 C_2\right\}. \tag{30.21}$$

The coefficient C_2 is defined by (30.15a). Up to terms in τ^{-2} we get now

$$\sigma = t_0 + t_0(1 - t_0^2) \frac{1}{\tau} + t_0(1 - t_0^2)(2 - C_2 - 2t_0^2) \frac{1}{\tau^2}. \tag{30.22}$$

In the nearest-neighbour case $C_2 = (1 + \nu)/\nu$ (ν: number of nearest neighbours) and thus

$$\sigma = t_0 + t_0(1 - t_0^2) \frac{1}{\tau} + t_0(1 - t_0^2) \left(\frac{\nu - 1}{\nu} - 2t_0^2\right) \frac{1}{\tau^2}. \tag{30.23}$$

We have written (30.20) in this form to ease the comparison with Opechowski's results which were obtained by the standard thermodynamic perturbation theory (there is no doubt about the applicability of this method at high temperatures). In our notation the magnetisation evaluated from (30.23) differs from Opechowski's result (1937) by a quantity of order $1/\nu_T{}^2$:

$$\sigma_{(30.23)} - \sigma_{\text{Opech.}} = \frac{(1 - t_0^2)^2}{\nu_T{}^2}, \tag{30.24}$$

so that also here there is very satisfactory agreement between our approximate results and the exact ones.

Equation (30.2) gives thus, indeed, very satisfactory results for the magnetisation for all temperatures.

We must note especially that (30.2) describes, in particular, also the phase transition from the ferromagnetic into the paramagnetic state. We remind ourselves in this connexion of the fact that the same was the case in our treatment of superconductivity considered in the preceding chapter. We see thus that in accordance with what we said in the Introduction the Green function method gives a well-defined possibility to start a study of phase changes.

Once we know the correlation function $\langle b^+(\vec{f})b(\vec{g})\rangle$ it would be easy to evaluate also other thermodynamic quantities, for instance, the average energy, and so on *. We shall not discuss this any further here.

We must note that the solution studied here exists for arbitrary fields $\mathcal{H}$ only if the exchange integral is positive.

If $A < 0$ (antiferromagnetic case) the solution considered above exists only provided the field is sufficiently strong, $\mu_B\mathcal{H} > 2\sigma|A'(0)|$. In the opposite case, the spectral function $J(E)$ would be negative, and this is impossible by virtue of (4.2) (this would mean in the present case that the average occupation number n would be negative). In that case when $A < 0$, $\mu_B\mathcal{H} < 2\sigma|A'(0)|$ we need modify somewhat the scheme described here and introduce two or several sublattices (Fu-Cho 1960a, b) by analogy with the procedure in the approximate second-quantisation method or in the molecular-field theory (see, for instance, ter Haar and Lines 1962).

If we wish to proceed further to the second approximation, we should write down the equation for the two-particle Green function and write down an approximate expression for the three-particle Green function occurring in this equation in terms of lower order Green functions (compare Tahir-Kheli and ter Haar 1962b).

* See, for instance, Tahir-Kheli and ter Haar 1962a, b (Note by translator).

31. FERROMAGNETIC RESONANCE

It is well-known that ferromagnetic resonance consists in the absorption of energy from a variable radio-frequency field by a system of spins which are connected through exchange forces and which are situated in a constant magnetic field. The absorption curve has a more or less steep maximum at some frequency (the resonance frequency) which depends mainly on the magnitude of the constant external field. Both the classical and the quantum-mechanical aspects of the theory of ferromagnetic resonance have been studied extensively by many authors.

We shall study here the problem of the ferromagnetic resonance frequency using the general method of section 14. This will enable us to obtain formulae suitable for all temperatures by using the results of the preceding section.

In studying ferromagnetic resonance we must be able to find the changes in the average magnetisation components $\delta\tilde{m}_i(x_0)$ $(i = 1,2,3)$ caused by the radio-frequency field $h_i(x_0)$, as they give us the complex susceptibility

$$\delta\tilde{m}(x_0) = \chi\, \vec{h}(x_0) \,, \tag{31.1}$$

which determines the transfer of energy from the radio-frequency field to the spin system. Noting that

$$\delta\tilde{m}_i(x_0) = \mu_B \delta\tilde{S}_i(\vec{f}, x_0) \,, \tag{31.2}$$

we see that the problem is reduced to evaluating the average changes in the spin operators $\delta\tilde{S}_i(\vec{f}, x_0)$ - which is independent of $\vec{f}$ because of translational invariance.

If there is an external radio-frequency field present the Hamiltonian of the system can be written in the form

$$H = H_0 + \Delta H(x_0) \,. \tag{31.3}$$

The operator ΔH describes the interaction between the system and the radio-frequency field, and H_0 includes all other interactions such as exchange interactions or the interaction with the external constant magnetic field.

To fix our ideas, we assume that the constant magnetic field is along the z-axis, and that the field $\vec{h}$ lies in the x, y-plane. We assume, moreover, as usual, that the wavelengths of the radio-frequency field are large compared with the dimensions of the sample so that we may assume that the field is uniform in space. We have then for $\Delta H(x_0)$

$$\Delta H(x_0) = -\mu_B \sum_{\beta, \vec{f}} h_\beta(x_0)\, S_\beta(x_0, \vec{f}) \,. \tag{31.4}$$

* Tyablikov 1960a.

Here and henceforth in this chapter Greek indices take on the values 1 and 2; this differs from the convention used elsewhere in this book. We write $h_\beta(x_0)$ in the form

$$h_\beta(x_0) = \sum_\omega h_\beta(\omega)\, e^{-i\omega x_0 - \epsilon|x_0|} . \tag{31.5}$$

The Hamiltonian (31.4) becomes then a sum of standard expressions of the form (14.1), and we can use for the magnetic susceptibility the general formula (14.10). We need only adapt it to fit the present situation by taking for C_2 and C_1 two components of the spin angular momentum.

Let us now consider the case of a plane-polarised radio-frequency field. As we shall restrict ourselves here to the approximation which is linear in the external field, we can take (31.4) to be as follows

$$\Delta H(x_0) = -\mu_B\, e^{-i\omega x_0} \sum_{\beta,\vec{f}} h_\beta\, S_\beta(\vec{f}) . \tag{31.6}$$

We get then from (14.10)

$$\chi_{\beta\gamma} = -\mu_B^2 \sum_{\vec{f}} 2\pi \ll S_\beta(\vec{g}) | S_\gamma(\vec{f}) \gg_{r, E=\omega} . \tag{31.7}$$

To evaluate the magnetic susceptibility we must thus find the Fourier transform of the Green function $\ll S_\beta(\vec{g}) | S_\gamma(\vec{f}) \gg$.

It is convenient to change over from the spin operators to the Pauli operators (see appendix II)

$$S_1(\vec{f}) = b(\vec{f}) + b^+(\vec{f}) , \quad S_2 = i\,[b^+(\vec{f}) - b(\vec{f})] , \quad S_3 = 1 - 2\,n(\vec{f}) . \tag{31.8}$$

We then get from (31.7)

$$\begin{aligned}
\chi_{11} &= 2\pi\mu_B^2 \sum_{\vec{f}} \{G_{11}(\vec{g},\vec{f}) + G_{22}(\vec{g},\vec{f}) + G_{21}(\vec{g},\vec{f}) + G_{12}(\vec{g},\vec{f})\}_{E=\omega} , \\
\chi_{21} &= 2\pi i\mu_B^2 \sum_{\vec{f}} \{-G_{11}(\vec{g},\vec{f}) + G_{22}(\vec{g},\vec{f}) + G_{21}(\vec{g},\vec{f}) - G_{12}(\vec{g},\vec{f})\}_{E=\omega} , \\
\chi_{12} &= 2\pi i\mu_B^2 \sum_{\vec{f}} \{\ G_{11}(\vec{g},\vec{f}) - G_{22}(\vec{g},\vec{f}) + G_{21}(\vec{g},\vec{f}) - G_{12}(\vec{g},\vec{f})\}_{E=\omega} , \\
\chi_{22} &= 2\pi\mu_B^2 \sum_{\vec{f}} \{\ G_{11}(\vec{g},\vec{f}) + G_{22}(\vec{g},\vec{f}) - G_{21}(\vec{g},\vec{f}) - G_{12}(\vec{g},\vec{f})\}_{E=\omega} .
\end{aligned} \tag{31.9}$$

We have used here the notation (compare (29.3))

$$G_{11}(\vec{g},\vec{f}) = \ll b(\vec{g}) | b^+(\vec{f}) \gg^{(-)} , \quad G_{22}(\vec{g},\vec{f}) = \ll b^+(\vec{g}) | b(\vec{f}) \gg^{(-)} , \tag{31.10}$$

$$G_{21}(\vec{g},\vec{f}) = \ll b^+(\vec{g}) | b^+(\vec{f}) \gg^{(-)} , \quad G_{12}(\vec{g},\vec{f}) = \ll b(\vec{g}) | b(\vec{f}) \gg^{(-)} . \tag{31.11}$$

The functions G_{11}, G_{12}, G_{21}, and G_{22} are determined by solving the

appropriate equations, the form of which depends on the actual form of the Hamiltonian H_0. For an isotropic ferromagnet in a constant field which is along the z-axis, we have

$$H_0 = -\mu_B \mathcal{H} \sum_{\vec{f}} S_z(\vec{f}) - \tfrac{1}{2} \sum_{\vec{f}_1,\vec{f}_2} A(\vec{f}_1-\vec{f}_2)(\vec{S}(\vec{f}_1)\cdot\vec{S}(\vec{f}_2)) \,. \qquad (31.12)$$

For a finite specimen we must also take into account the demagnetising action of its boundaries. The classical expression for the demagnetisation energy (per atom) is for an ellipsoidal specimen of the form

$$H_{\text{demagn}} = \frac{1}{2N} \sum_{i=1}^{3} N_i M_i^2 \,, \qquad (31.13)$$

where N is the number of lattice sites, N_i the demagnetisation factor, and M_i the i-th component of the magnetisation vector. To go from the classical to a quantum mechanical expression we shall take for the M_i the components of the total magnetic moment (Oguchi 1957):

$$M_i = \mu_B \sum_{\vec{f}} S_i(\vec{f}) \,. \qquad (31.14)$$

For an ellipsoidal specimen we get then for the Hamiltonian H_0 the sum of (31.12) and (31.13).

The demagnetisation part of the Hamiltonian in terms of the Pauli operators is

$$\begin{aligned} H_{\text{demagn}} = {} & \tfrac{1}{2} N N_3 \mu_B^2 - 2\mu_B^2 N_3 \sum_{\vec{f}} \mathfrak{n}(\vec{f}) + \frac{2\mu_B^2 N_3}{N} \sum_{\vec{f}_1,\vec{f}_2} \mathfrak{n}(\vec{f}_1)\,\mathfrak{n}(\vec{f}_2) \\ & + \frac{\mu_B^2}{2N}(N_1-N_2) \sum_{\vec{f}_1,\vec{f}_2} [b(\vec{f}_1)\, b(\vec{f}_2) + b^+(\vec{f}_1)\, b^+(\vec{f}_2)] \\ & + \frac{\mu_B^2}{N}(N_1+N_2) \sum_{\vec{f}_1,\vec{f}_2} b^+(\vec{f}_1)\, b(\vec{f}_2) + O(\tfrac{1}{N}) \,. \end{aligned} \qquad (31.15)$$

We shall consider the case of an unbounded medium and that of an ellipsoidal specimen separately.

a. *Unbounded medium.* In this case the Hamiltonian H_0 is given by (31.12) and we can immediately use the results of section 29 to determine the Green functions. In the first approximation we have from (29.10) and (29.11)

$$G_{11}(\vec{g},\vec{f};E) = -\frac{\sigma}{2\pi} \cdot \frac{1}{N} \sum_{\vec{k}} e^{i(\vec{g}-\vec{f}).\vec{k}} \frac{1}{E - W(\vec{k})} \,, \qquad (31.16)$$

$$G_{11}(\vec{g},\vec{f};E) = -\frac{\sigma}{2\pi}\cdot\frac{1}{N}\sum_{\vec{k}} e^{i(\vec{g}-\vec{f}\cdot\vec{k})}\frac{1}{E - W(\vec{k})}, \tag{31.16}$$

$$G_{22}(\vec{g},\vec{f};E) = G_{11}(\vec{g},\vec{f};-E)\ , \tag{31.17}$$

$$G_{21}(\vec{g},\vec{f};E) = G_{12}(\vec{g},\vec{f};E) = 0\ , \tag{31.18}$$

$$W(\vec{k}) = 2\mu_B\mathcal{H} + \sigma\,[2A'(0) - 2A'(\vec{k})]\ . \tag{31.19}$$

As the Fourier transform of the retarded Green functions are defined only for Im $E > 0$ (see section 3) we shall in the following put everywhere

$$\frac{1}{E - W(\vec{k})} = \mathcal{P}\frac{1}{E - W(\vec{k})} - \pi i\delta\,[E - W(\vec{k})]\ . \tag{31.20}$$

Substituting (31.16) to (31.18) into (31.9) and using (31.20) we find

$$\chi_{\beta\gamma} = \chi'_{\beta\gamma} + i\,\chi''_{\beta\gamma}\ , \quad \chi_{11} = \chi_{22}\ , \quad \chi_{12} = -\chi_{21}\ , \tag{31.21}$$

$$\chi'_{11} = \chi_0\,\mathcal{P}\,[1 - (\frac{\omega}{E_0})^2]^{-1}\ , \quad \chi''_{11} = \frac{\pi}{2}\chi_0 E_0\,\delta(\omega - E_0)\ , \tag{31.22}$$

$$\chi'_{21} = \frac{\pi}{2}\chi_0 E_0\,\delta(\omega - E_0)\ , \quad \chi''_{21} = -\frac{\omega}{E_0}\chi_0\,\mathcal{P}\,[1 - (\frac{\omega}{E_0})^2]^{-1}\ ,$$

where

$$\chi_0 = \frac{2\mu_B^2\sigma}{E_0} = \frac{\mu_B\sigma}{\mathcal{H}}\ , \quad E_0 = 2\mu_B\mathcal{H}\ . \tag{31.23}$$

Equation (31.23) determines the resonance frequency E_0 for an unbounded medium. It is, however, known experimentally that the shape of the sample is of great importance for the resonance condition and (31.23) is thus basically of methodological interest only.

b. *Ellipsoidal samples.* The Hamiltonian is in this case the sum of (31.12) and (31.13) and we must determine the Green functions again. We get their equations of motion in the usual way. As in section 29 we break off the chain of equations at the first one by putting

$$\ll\mathfrak{N}(\vec{g})\,b(\vec{g}')\,|\,b^+(\vec{f})\gg^{(-)} \approx \langle\mathfrak{N}(\vec{g})\rangle\ll b(\vec{g}')\,|\,b^+(\vec{f})\gg^{(-)} = n\,G_{11}(\vec{g}',\vec{f})\ , \tag{31.24}$$

$$\ll\mathfrak{N}(\vec{g})\,b^+(\vec{g}')\,|\,b^+(\vec{f})\gg^{(-)} \approx \langle\mathfrak{N}(\vec{g})\rangle\ll b^+(\vec{g}')\,|\,b^+(\vec{f})\gg^{(-)} = n\,G_{21}(\vec{g}',\vec{f})\ . \tag{31.25}$$

We get then for the G the following set of equations

$$i\frac{\partial G_{11}(\vec{g},\vec{f};t)}{\partial t} = -\sigma\Delta(\vec{g}-\vec{f})\,\delta(x_0-x_0') + \frac{\sigma\mu_B^2}{N}(N_1-N_2)\sum_{\vec{g}'} G_{21}(\vec{g}',\vec{f})$$
$$+ \{2\mu_B\mathcal{H} + \sigma\,[2A'(0) - 2\,\mu_B^2 N_3]\}\,G_{11}(\vec{g},\vec{f})$$
$$- \sum_{\vec{g}'}\sigma\,[2A(\vec{g}-\vec{g}') - \frac{\mu_B^2}{N}(N_1+N_2)]\,G_{11}(\vec{g}',\vec{f})\,, \qquad (31.26)$$

$$i\frac{\partial G_{21}(\vec{g},\vec{f};t)}{\partial t} = -\frac{\sigma\mu_B^2}{N}(N_1-N_2)\sum_{\vec{g}'} G_{11}(\vec{g}',\vec{f})$$
$$- \{2\mu_B\mathcal{H} + \sigma\,[2A'(0) - 2\mu_B^2 N_3]\}\,G_{21}(\vec{g},\vec{f})$$
$$+ \sum_{\vec{g}'}\sigma\,[2A(\vec{g}-\vec{g}') - \frac{\mu_B^2}{N}(N_1+N_2)]\,G_{21}(\vec{g}',\vec{f})\,.$$

If we perform the usual Fourier transformation

$$G_{11}(\vec{g},\vec{f};t) = \frac{1}{N}\sum_{\vec{k}} e^{i(\vec{g}-\vec{f}\cdot\vec{k})}\int_{-\infty}^{+\infty} dE\; G_{11}(\vec{k},E)\,e^{-iEt}\,,$$
$$G_{21}(\vec{g},\vec{f};t) = \frac{1}{N}\sum_{\vec{k}} e^{i(\vec{g}-\vec{f}\cdot\vec{k})}\int_{-\infty}^{+\infty} dE\; G_{21}(\vec{k},E)\,e^{-iEt}\,, \qquad (31.27)$$

we get an algebraic set of equations:

$$[E - W'(\vec{k})]\,G_{11}(\vec{k},E) - \Delta(\vec{k})\,\sigma\mu_B^2(N_1-N_2)\,G_{21}(\vec{k},E) = -\frac{\sigma}{2\pi}\,,$$
$$\Delta(\vec{k})\,\sigma\mu_B^2(N_1-N_2)\,G_{11}(\vec{k},E) + [E + W'(\vec{k})]\,G_{21}(\vec{k},E) = 0\,. \qquad (31.28)$$

Here

$$W'(\vec{k}) = 2\mu_B(\mathcal{H} - \sigma\mu_B N_3) + \sigma\,[2A'(0) - 2A'(\vec{k})] + \sigma\mu_B^2(N_1+N_2)\,\Delta(\vec{k})\,. \qquad (31.29)$$

We shall solve (31.28) separately for the case $\vec{k} \neq 0$, and the case $\vec{k} = 0$.

If $\vec{k} \neq 0$, we get from (31.28)

$$[E - W'(\vec{k})]\,G_{11}(\vec{k},E) = -\frac{\sigma}{2\pi}\,, \qquad G_{21}(\vec{k},E) = 0\,,$$
$$W'(\vec{k}) = 2\mu_B(\mathcal{H} - \sigma\mu_B N_3) + \sigma\,[2A'(0) - 2A'(\vec{k})]\,. \qquad (31.30)$$

We can use $G_{11}(\vec{k},E)$ to get an equation for the as yet unknown quantity σ. By complete analogy with (29.19) we get

$$\frac{1}{\sigma} = \frac{v}{(2\pi)^3} \int \coth \tfrac{1}{2}\beta W'(\vec{k})\, d^3\vec{k} \,. \tag{31.31}$$

One verifies easily that this equation like (29.19) gives a very satisfactory interpolation formula for all temperatures. The quantity $W'(\vec{k})$ determines the elementary excitation spectrum in the system and can not be negative (if we assume that $W'(\vec{k})$ can take on negative values we are led to a contradiction: $n < 0$). The solution (31.30) is thus possible only if $W'(\vec{k}) \geq 0$ for all $\vec{k}$. As the second term in $W'(\vec{k})$ is non-negative, we can get the solution considered here only in sufficiently high fields:

$$\mathcal{H} - \sigma\mu_B N_3 \geq 0 \,. \tag{31.32}$$

The physical meaning of this relation is obvious: the external field must "overcome" the demagnetisation influence of the boundaries.

Consider now the case when $\vec{k} = 0$. We get then from (31.28)

$$\begin{aligned} (E-E_0)\, G_{11}(0,E) - \sigma\mu_B^2(N_1-N_2)\, G_{21}(0,E) &= -\frac{\sigma}{2\pi} \,, \\ \sigma\mu_B^2(N_1-N_2)\, G_{11}(0,E) + (E+E_0)\, G_{21}(0,E) &= 0 \,, \end{aligned} \tag{31.33}$$

where

$$E_0 = 2\mu_B\mathcal{H} + \sigma\mu_B^2(N_1+N_2-2N_3) \,. \tag{31.34}$$

We now find easily

$$G_{11}(0,E) = -\frac{\sigma}{2\pi} \cdot \frac{E_0 + E}{E^2 - E_r^2} \,, \qquad G_{21}(0,E) = \frac{\sigma}{2\pi} \cdot \frac{\sigma\mu_B^2(N_1-N_2)}{E^2 - E_r^2} \tag{31.35}$$

and similarly

$$G_{22}(0,E) = -\frac{\sigma}{2\pi} \cdot \frac{E_0 - E}{E^2 - E_r^2} \,, \qquad G_{12}(0,E) = G_{21}(0,E) \,, \tag{31.35a}$$

where

$$E_r = \sqrt{A_1 A_2} \equiv 2\mu_B \sqrt{\{\mathcal{H} + \sigma\mu_B(N_1-N_3)\}\{\mathcal{H} + \sigma\mu_B(N_2-N_3)\}} \,. \tag{31.36}$$

If we now substitute (31.35) and (31.35a) into (31.9) and use, as before, (31.20) we get finally the following expressions for the components of the susceptibility tensor:

$$\begin{aligned} &\chi_{\beta\gamma} = \chi'_{\beta\gamma} + i\,\chi''_{\beta\gamma} \,, \qquad \chi_{12} = -\chi_{21} \,, \qquad \chi_0 = \frac{2\sigma\mu_B^2}{E_r} \,, \\ &\chi'_{11} = \chi_0 \sqrt{\frac{A_2}{A_1}}\, \mathcal{P}\, \frac{1}{1 - \omega^2/E_r^2} \,, \qquad \chi''_{11} = \frac{\pi\chi_0}{2} A_2\, \delta(\omega - E_r) \,, \\ &\chi'_{21} = \frac{\pi\chi_0}{2} E_r\, \delta(\omega - E_r) \,, \qquad \chi''_{21} = -\frac{\omega\chi_0}{E_r}\, \mathcal{P}\, \frac{1}{1 - \omega^2/E_r^2} \,, \\ &\chi'_{22} = \chi_0 \sqrt{\frac{A_1}{A_2}}\, \mathcal{P}\, \frac{1}{1 - \omega^2/E_r^2} \,, \qquad \chi''_{22} = \frac{\pi\chi_0}{2} A_1\, \delta(\omega - E_r) \,. \end{aligned} \tag{31.37}$$

The quantity χ'' characterises the absorption of energy from the radio-frequency field by the spin system. In the approximation considered this absorption occurs at a frequency of the radio-frequency field equal to E_r; at the same time the spin system is "swung round" by the radio-frequency field. In other words there occurs resonance when the frequency ω of the external field is the same as the eigen-frequency E_r of the system.

Kittel (1948) was the first to evaluate the value of the resonance frequency, taking the influence of the demagnetisation factors, N_i, into account. He obtained the following equation (in our notation)

$$E_r = 2\mu_B \sqrt{\{\mathcal{H} + \mu_B(N_1 - N_3)\}\{\mathcal{H} + \mu_B(N_2 - N_3)\}}. \qquad (31.38)$$

The values of the resonance frequencies obtained from this equation turned out to be in good agreement with the experimental data.

Equation (31.36) is a generalisation of Kittel's formula (31.38) which is valid at all temperatures.

We must note that the ferromagnetic resonance line in our case turns out to be delta-function shaped. This is connected with the fact that in the present approximation the Green functions have poles on the real axis only, and there is thus no damping of the excitations. To get the damping which determines the shape and the width of the resonance line, we need consider better approximations (spin-wave spin-wave scattering processes). One must, however, bear in mind that the actual spin-wave damping (and thus the broadening of the absorption lines) is connected also with a whole lot of other factors: magnetic anisotropy of the crystal, spin-wave - lattice interaction, spin-wave - conduction electron interaction, and so on. It is as yet far from clear which mechanism is the most important one for the spin-wave damping.

32. GENERAL RELATIONS FOR FERROMAGNETIC RESONANCE *

We applied the Green function method to the theory of ferromagnetic resonance in the preceding section. We wrote down expressions for the susceptibility χ in terms of the Green functions for the given Hamiltonian of the spin system, H_0. To obtain specific results we used then a well-defined model representation for the spin system Hamiltonian H_0 and also introduced some approximations in decoupling the chain of Green function equations.

In the following we shall consider the problem of ferromagnetic resonance in the linear approximation under more general conditions and we shall attempt to obtain certain conclusions about the behaviour of the susceptibility under the most general assumptions possible

* Tyablikov 1960b.

about the Hamiltonian H_0 of the spin system itself. We shall base our considerations only upon the analytical properties of the retarded Green functions, in terms of which we have an expression for χ, and on the form of the operator of the interaction between the spin system and the radio-frequency field. We shall restrict ourselves to our earlier statement of the problem, where we assumed that the constant field was along the z-axis and that the (plane-polarised) radio-frequency field was situated in the xy-plane. We note, moreover, easily that equations (31.9) for the susceptibility are not restricted by any specific assumption about the form of the spin system Hamiltonian.

It is convenient for what follows to write the interaction Hamiltonian (31.4) somewhat differently:

$$\Delta H(x_0) = \sum_{\omega>0} e^{-\varepsilon|x_0|} \{V_\omega e^{-i\omega x_0} + V_\omega^+ e^{i\omega x_0}\}, \qquad (32.1)$$

where

$$V_\omega = -\mu_B \sum_{\beta,\vec{f}} h_\beta(\omega) S_\beta(x_0, \vec{f}); \quad V_\omega^+ = V_{-\omega}.$$

For the average change in the magnetisation vector

$$M_i = \mu_B \sum_{\vec{f}} S_i(x_0, \vec{f})$$

we get then from (14.10)

$$\delta\tilde{M}_\beta(x_0) = \sum_{\omega>0,\gamma} \{X_{\beta\gamma}(\omega) h_\gamma(\omega) e^{-i\omega x_0} + X_{\beta\gamma}(-\omega) h_\gamma^+(\omega) e^{i\omega x_0}\}. \qquad (32.2)$$

The components $X_{\beta\gamma}$ are connected with the $\chi_{\beta\gamma}$, which are given by (31.9) through the obvious relations

$$X_{\beta\gamma} = \sum_{\vec{g}} \chi_{\beta\gamma}(\omega, \vec{g}). \qquad (32.3)$$

The peculiar features of the different problems such as the form of the Hamiltonian or the shape of the specimen enter into the consideration through the $G_{\beta\gamma}$, as can be seen from (31.9). We shall not be interested in the present section in determining them directly, but we shall instead concentrate on elucidating those general properties of the susceptibility tensor which are not connected with a specific problem.

Instead of the $b(\vec{f})$ and $b^+(\vec{f})$ we introduce new operators

$$B = \sum_{\vec{f}} b(\vec{f}), \quad B^+ = \sum_{\vec{f}} b^+(\vec{f}), \quad N = \sum_{\vec{f}} b^+(\vec{f}) b(\vec{f}), \qquad (32.4)$$

and accordingly the Green functions

$$G_{11}(E) = \ll B \mid B^+ \gg_E^{(-)}, \qquad G_{12}(E) = \ll B \mid B \gg_E^{(-)},$$
$$G_{21}(E) = \ll B^+ \mid B^+ \gg_E^{(-)}, \qquad G_{22}(E) = \ll B^+ \mid B \gg_E^{(-)}, \tag{32.5}$$

where E is a complex variable. We have not indicated in (32.5) with which Green function we are concerned, as the retarded and advanced Green functions in the complex plane can be considered to be one analytical function (see section 3). We need distinguish between them only for real values of E ($E = \omega$) and in that case we must attach a superscript "r".

Let us now write the susceptibility tensor X in the standard form

$$X(\omega) = \begin{Vmatrix} X_1(\omega) + X_2(\omega) & i\,[Y_1(\omega) + Y_2(\omega)] & 0 \\ -i\,[Y_1(\omega) - Y_2(\omega)] & X_1(\omega) - X_2(\omega) & 0 \\ 0 & 0 & X_0 \end{Vmatrix}. \tag{32.6}$$

We have put here

$$X_1(\omega) = u\,\{G_{11}^r(\omega) + G_{22}^r(\omega)\}, \qquad X_2(\omega) = u\,\{G_{12}^r(\omega) + G_{21}^r(\omega)\},$$
$$Y_1(\omega) = u\,\{G_{11}^r(\omega) - G_{22}^r(\omega)\}, \qquad Y_2(\omega) = u\,\{-G_{12}^r(\omega) + G_{21}^r(\omega)\}, \tag{32.7}$$
$$u = 2\pi\mu_B^2.$$

We shall now take into account that for Green functions of this form for real values of the argument ($E = \omega$) (3.31) holds, and that we have thus

$$\ll A \mid B \gg_\omega^r = [\ll A^+ \mid B^+ \gg_{-\omega}^r]^+.$$

We have thus

$$G_{11}^r(\omega) = [G_{11}^r(-\omega)]^+, \qquad G_{12}^r(\omega) = [G_{21}^r(-\omega)]^+. \tag{32.8}$$

From (32.7) and (32.8) we get the well-known relations (Landau and Lifshitz 1959, Kubo 1957)

$$X_{\beta\gamma}(\omega) = X_{\beta\gamma}^+(-\omega), \tag{32.9}$$

$$X_1(\omega) = X_1^+(-\omega), \qquad X_2(\omega) = X_2^+(-\omega),$$
$$Y_1(\omega) = -Y_1^+(-\omega), \qquad Y_2(\omega) = -Y_2^+(-\omega). \tag{32.10}$$

Kubo (1957) obtained these results by a method which is closely akin to the Green function method (for details see Zubarev 1960 and section 14).

From this we get for the real ($X'_{\beta\gamma}$) and imaginary ($X''_{\beta\gamma}$) parts of the susceptibility

$$X'_{\beta\gamma}(\omega) = X'_{\beta\gamma}(-\omega) , \qquad X''_{\beta\gamma}(\omega) = - X''_{\beta\gamma}(-\omega) , \tag{32.11}$$

$$X'_{12}(\omega) = X'_{12}(-\omega) , \qquad X''_{12}(\omega) = - X''_{12}(-\omega) , \tag{32.12}$$

$$Y'_{12}(\omega) = - Y'_{12}(-\omega) , \qquad Y''_{12}(\omega) = Y''_{12}(-\omega) . \tag{32.13}$$

We assume now that the equations of motion for B and B^+ are invariant under time reversal, that is, invariant under the transformation

$$t \to - t , \quad i \to - i . \tag{32.14}$$

We have then apart from (32.8) and (32.9) to (32.13) which are always valid yet another connexion between the $G^r_{\beta\gamma}$: for real E we have from (3.37)

$$\ll A | B \gg^r_\omega = \ll B^+ | A^+ \gg^r_\omega ,$$

and hence

$$G^r_{12}(\omega) = G^r_{21}(\omega) , \tag{32.15}$$

and also

$$Y_2(\omega) = 0 , \qquad X_2(\omega) = 2u\, G^r_{12}(\omega) . \tag{32.16}$$

Let us consider in somewhat more detail the behaviour of the susceptibility in the resonance region. This is clearly basically determined by the poles of the $G_{\beta\gamma}$ given by (32.5). We shall therefore consider the $G_{\beta\gamma}$ in the complex plane.

Following an earlier paper (Tyablikov 1960b) we introduce a matrix $G(E)$

$$G(E) = \begin{pmatrix} G_{11}(E) & G_{12}(E) \\ G_{21}(E) & G_{22}(E) \end{pmatrix} , \tag{32.17}$$

where the $G_{\beta\gamma}$ are defined by (32.7).

In the complex plane (3.29) holds and we have thus:

$$\ll A | B \gg_E = \ll B | A \gg_{-E} ,$$

and thus for the elements of the matrix (32.17)

$$G_{11}(E) = G_{22}(-E) , \qquad G_{12}(E) = G_{21}(-E) . \tag{32.18}$$

We introduce a matrix F which is the inverse of the matrix G. One can easily shew that its elements $F_{\beta\gamma}(E)$ are connected by relations similar to (32.18). We can express the $G_{\beta\gamma}$ in terms of the $F_{\beta\gamma}$:

$$G_{11}(E) = \frac{F_{22}(E)}{\Delta(E)} , \qquad G_{12}(E) = - \frac{F_{12}(E)}{\Delta(E)} , \tag{32.19}$$

where

$$\Delta(E) = F_{11}(E)\, F_{22}(E) - F_{12}(E)\, F_{21}(E) = \Delta(-E) . \tag{32.20}$$

Let $G(E)$ have a pole at $E = E_R$. Since $F(E)$ is regular in this point, E_R is a root of the equation $\Delta(E) = 0$. From (32.20) it follows that $-E_R$ will also be a root of this equation. We have thus

$$\Delta(E) = (E^2 - E_R^2)\, A(E) , \qquad A(-E) = A(E) , \tag{32.21}$$

where $A(E)$ is a function of E.

If we now define the following functions

$$F_{11}(E) = F_{22}(-E) \equiv F(E) , \qquad F_{12}(E) = F_{12}(-E) \equiv \Phi_1(E) ,$$

$$F_{21}(E) = F_{21}(-E) \equiv \Phi_2(E) , \tag{32.22}$$

and use (32.21), we get from (32.19)

$$G_{11}(E) = \frac{F(-E)}{2E_R\, A(E)}\, R(E) , \qquad G_{12}(E) = -\frac{\Phi_1(E)}{2E_R\, A(E)}\, R(E) , \ \ldots \tag{32.23}$$

where

$$R(E) = \frac{1}{E - E_R} - \frac{1}{E + E_R} . \tag{32.24}$$

Substituting (32.23) into (32.7), we get for $X_1(E)$, ...

$$X_1(E) = u\, \frac{F(-E) + F(E)}{2E_R\, A(E)}\, R(E) , \qquad X_2(E) = -u\, \frac{\Phi_1(E) + \Phi_2(E)}{2E_R\, A(E)}\, R(E) ,$$

$$Y_1(E) = u\, \frac{F(-E) - F(E)}{2E_R\, A(E)}\, R(E) , \qquad Y_2(E) = u\, \frac{\Phi_1(E) - \Phi_2(E)}{2E_R\, A(E)}\, R(E) , \tag{32.25}$$

where R and A are defined by (32.24) and (32.21).

The quantities $X_1, \ldots, Y_2$ are interconnected because of (32.19) and (32.20) through the relation

$$X_1^2(E) - X_2^2(E) - Y_1^2(E) + Y_2^2(E) = \frac{(4\pi\mu_B^2)^2}{2E_R\, A(E)}\, R(E) , \tag{32.26}$$

or,

$$X_{11}(E)X_{22}(E) - X_{12}(E)X_{21}(E) = \frac{(4\pi\mu_B^2)^2}{2E_R\, A(E)}\, R(E) . \tag{32.27}$$

Let us now consider the behaviour of $X_1(E)$ for values of E near E_R. As the factors of $R(E)$ in (32.25) are regular functions of E for values sufficiently close to E_R, we can in these factors replace E by E_R. This will not introduce a large error, as we are taking the singularity exactly into account by considering $R(E)$ separately. We can thus write (32.25) approximately in the following form for E-values close to E_R:

$$X_1(E) \approx u\, \frac{F(-E_R) + F(E_R)}{2E_R\, A(E_R)}\, R(E) , \ \ldots$$

Moreover, if we use the fact that

$$\Delta(E_R) = F(-E_R)\, F(E_R) - \Phi_1(E_R)\, \Phi_2(E_R) = 0 ,$$

we get finally

$$X_1(E) \approx C(1+K_1K_2)\ R(E)\ , \qquad X_2(E) \approx -C(K_1+K_2)\ R(E)\ ,$$
$$Y_1(E) \approx C(1-K_1K_2)\ R(E)\ , \qquad Y_2(E) \approx\ C(K_1-K_2)\ R(E)\ , \tag{32.28}$$

where

$$K_1 = \frac{\Phi_1(E_R)}{F(-E_R)}\ , \qquad K_2 = \frac{\Phi_2(E_R)}{F(-E_R)}\ , \qquad C = u\,\frac{F(-E_R)}{2E_R\ A(E_R)}\ . \tag{32.29}$$

If the equations of motion for B and B^+ are invariant under time-reversal, we have

$$\Phi_2(E) = \Phi_1(E)\ , \qquad K_2 = K_1\ , \qquad Y_2 = 0\ . \tag{32.30}$$

The magnetic susceptibility is defined through (32.7) in terms of the values of the retarded Green functions on the real axis. We shall now obtain the equations which correspond to (32.25) to (32.30) for real E and E_R.

We first of all use (32.8). By proceeding in the same way as before we get

$$G^r_{11}(\omega) = \frac{F^r_{22}(\omega)}{\Delta_r(\omega)} = \frac{[F^r(-\omega)]^+}{2\omega_R\ A^r(\omega)}\ R_r(\omega)\ ,$$

$$G^r_{12}(\omega) = \frac{-\ F^r_{21}(\omega)}{\Delta_r(\omega)} = \frac{[\Phi^r(-\omega)]^+}{2\omega_R\ A^r(\omega)}\ R_r(\omega)\ , \ \ldots\ , \tag{32.31}$$

where

$$\Delta_r(\omega) = \Delta^+_r(-\omega) = (\omega^2-\omega^2_R)\ A_r(\omega)\ ,$$

$$\Delta_r(\omega) = F^r(\omega)\ [F^r(-\omega)]^+ - \Phi^r(\omega)\ [\Phi^r(-\omega)]^+\ , \tag{32.32}$$

$$A^r(\omega) = [A^r(-\omega)]^+\ ,$$

$$R_r(\omega) = \lim_{\varepsilon\to 0}\ \{\frac{1}{\omega - \omega_R + i\varepsilon} - \frac{1}{\omega + \omega_R + i\varepsilon}\}\ , \tag{32.33}$$

and where ω_R is a pole of G on the real axis. Finally,

$$F^r(\omega) \equiv F^r_{11}(\omega) = [F^r_{22}(-\omega)]^+\ , \qquad \Phi^r(\omega) \equiv F^r_{12}(\omega) = [F^r_{21}(-\omega)]^+ \tag{32.34}$$

are the elements of the matrix $F_{\beta\gamma}(\omega)$.

We then get

$$X_1(\omega) = u\frac{F^r(\omega) + [F^r(-\omega)]^+}{2\omega_R A^r(\omega)} R_r(\omega) ,$$

$$X_2(\omega) = -u\frac{\Phi^r(\omega) + [\Phi^r(-\omega)]^+}{2\omega_R A^r(\omega)} R_r(\omega) ,$$

$$Y_1(\omega) = -u\frac{-F^r(\omega) + [F^r(-\omega)]^+}{2\omega_R A^r(\omega)} R_r(\omega) , \qquad (32.35)$$

$$Y_2(\omega) = u\frac{\Phi^r(\omega) - [\Phi^r(-\omega)]^+}{2\omega_R A^r(\omega)} R_r(\omega) ,$$

$$X_1^2(\omega) - X_2^2(\omega) - Y_1^2(\omega) + Y_2^2(\omega) = \frac{(4\pi\mu_B^2)^2}{2\omega_R A^r(\omega)} R_r(\omega) , \qquad (32.36)$$

$$X_{11}(\omega) X_{22}(\omega) - X_{12}(\omega) X_{21}(\omega) = \frac{(4\pi\mu_B^2)^2}{2\omega_R A^r(\omega)} R_r(\omega) , \qquad (32.37)$$

and approximately, in the resonance region,

$$X_1(\omega) \approx C(1+K_1K_2) R_r(\omega) , \quad X_2(\omega) \approx -C(K_1+K_2) R_r(\omega) ,$$
$$Y_1(\omega) \approx C(1-K_1K_2) R_r(\omega) , \quad Y_2(\omega) \sim C(K_1-K_2) R_r(\omega) , \qquad (32.38)$$

where C, K_1, and C_2 are constants defined by

$$K_1 = \frac{\Phi^r(\omega_R)}{[F^r(-\omega_R)]^+} , \quad K_2 = \frac{[\Phi^r(-\omega_R)]^+}{[F^r(-\omega_R)]^+} , \quad C = u\frac{[F^r(-\omega_R)]^+}{2\omega_R A^r(\omega_R)} . \qquad (32.39)$$

If the equations of motion for B and B^+ are invariant under time-reversal, we have

$$[\Phi^r(\omega)]^+ = \Phi^r(-\omega) , \quad K_1 = K_2 , \quad Y_2(\omega) = 0 . \qquad (32.40)$$

The energy absorbed by the spin system from the radio-frequency field per unit time is numerically equal to the work done by the radio-frequency field on the system per unit time. This work can be defined as

$$\frac{d\tilde{A}(x_0)}{dx_0} = \sum_\beta h_\beta(x_0) \frac{d}{dx_0} \delta \tilde{M}_\beta(x_0) ,$$

or, if we use (32.1) and (32.2)

$$\frac{d\tilde{A}(x_0)}{dx_0} = -i \sum_{\substack{\beta,\gamma \\ \omega,\omega'>0}} \omega' \{h_\beta(\omega) e^{-i\omega x_0} + h_\beta^+(\omega) e^{i\omega x_0}\}$$

$$\times \{X_{\beta\gamma}(\omega') h_\gamma(\omega') e^{-i\omega' x_0} - X_{\beta\gamma}(-\omega') h_\gamma^+(\omega') e^{i\omega' x_0}\} .$$

If we use (32.9) we get from this for the average energy absorbed by the system per unit time the expression

$$w = \lim_{T\to\infty} \frac{1}{T} \int_0^T \frac{d\tilde{A}(x_0)}{dx_0}\, dx_0$$

$$= i \sum_{\substack{\beta,\gamma \\ \omega>0}} \omega \{X^+_{\beta\gamma}(\omega)\, h_\beta(\omega)\, h^+_\gamma(\omega) - X_{\beta\gamma}(\omega)\, h^+_\beta(\omega)\, h_\gamma(\omega)\} . \qquad (32.41)$$

For the case of a plane-polarised field which was considered in the preceding and in the present section we must put

$$h^+_\beta(\omega) = h_\beta(\omega) , \qquad \beta = 1,2 .$$

We then get from (32.41)

$$w = i \sum_{\substack{\beta,\gamma \\ \omega>0}} \omega \{X^+_{\beta\gamma}(\omega) - X_{\beta\gamma}(\omega)\}\, h_\beta(\omega)\, h_\gamma(\omega) \qquad (32.42)$$

$$= \sum_{\substack{\beta,\gamma \\ \omega>0}} 2\omega\, X''_{\beta\gamma}(\omega)\, h_\beta(\omega)\, h_\gamma(\omega) .$$

Landau and Lifshitz (1959), Kubo and Tomita (1954), and Kubo (1957) have derived this formula in a slightly different way. From this equation we get the well-known result that the absorption of energy from the radio-frequency field is determined by the imaginary part of the susceptibility tensor. The $X_{\beta\gamma}$ increase steeply in the neighbourhood of the poles of the Green function and the energy absorption shews a resonance behaviour.

From these results we see that one can obtain some information about the behaviour of the magnetic susceptibility near ferromagnetic resonance without making any specific assumptions about the Hamiltonian of the spin system. We shall now attempt to include in our considerations damping in the spin system. We shall thus assume that in some approximation the Green functions considered have poles E_R in the complex plane. (This can only be true approximately and can not be true always, as in general the Green functions may possess singularities of a much more complicated nature). If $\Gamma = \mathrm{Im}\, E_R$, Γ will clearly represent the damping in the spin system for processes described by the Green functions introduced by us (see section 3). Bearing in mind that as $\Gamma \to 0$ the corresponding formulae must go over into (32.31) to (32.33), we assume that the singular function (32.33) has the form

$$R_{\Gamma}(\omega) = \frac{1}{\omega - \omega_R + i\,\Gamma} - \frac{1}{\omega + \omega_R + i\,\Gamma}$$

$$= 2\omega_R \frac{\omega^2 - \omega_R^2 - \Gamma^2 - 2i\omega\Gamma}{(\omega^2 - \omega_R^2 - \Gamma^2)^2 + (2\omega\,\Gamma)^2}. \qquad (32.43)$$

Substituting (32.43) into (32.38) we get the results of the classical theory of the line width in ferromagnetic resonance (Bloembergen 1950). The only difference consists in that in the classical theory one assumes the presence of "frictional terms" in the equations of motion (Bloembergen 1950, Landau and Lifshitz 1935), while here we assumed the existence of singularities of a definite type in the Green functions.

Appendix I

INTRODUCTION TO QUANTUM FIELD THEORY

In this appendix we shall give the elements of quantum field theory techniques, inasfar as a knowledge of them is desirable for a clear understanding of the main part of this volume. One should, however, bear in mind that we do not present here a detailed presentation of the theory, but only a more or less plotted version of some of its results.

a. *Interaction representation and scattering matrix*

Let us consider a dynamic system with a Hamiltonian

$$H = H_0 + H_1 \ , \tag{I. 1}$$

where H_0 does not depend explicitly on the time. We shall assume that the eigenvalues and eigenfunctions of H_0 are known (they are indicated where necessary by an index n). In the Schrödinger representation we have the following equation of motion for the wave function of the whole system *

$$i \frac{\partial \hat{\Phi}}{\partial x_0} = \hat{H} \hat{\Phi} \ . \tag{I. 2}$$

We perform a canonical transformation by means of the unitary operator $U = \exp(-i\hat{H}_0 x_0)$, putting

$$\hat{\Phi}(x_0) = e^{-i\hat{H}_0 x_0} \hat{\Phi}'(x_0) \ . \tag{I. 3}$$

We get then for the wave function $\hat{\Phi}'$ in the new representation the equation

$$i \frac{\partial \hat{\Phi}'}{\partial x_0} = e^{i\hat{H}_0 x_0} \hat{H}_1 e^{-i\hat{H}_0 x_0} \hat{\Phi}' \ ,$$

that is,

$$i \frac{\partial \hat{\Phi}'}{\partial x_0} = H_1'(x_0) \hat{\Phi}' \ , \tag{I. 4}$$

$$H_1'(x_0) = e^{i\hat{H}_0 x_0} \hat{H}_1 e^{-i\hat{H}_0 x_0} \ . \tag{I. 5}$$

It is clear that equations such as (I. 5) determine also all other dynam-

* We have indicated operators in the Schrödinger representation by a caret: we shall also indicate in this way the wave functions in this representation.

ical variables in the new representation (indicated by a prime on the operators and wave functions). It is the so-called *interaction representation*. This nomenclature is connected with the fact that in most applications $\hat{H}_0$ describes a system of free particles and $\hat{H}_1$ the interaction between them. It is clear that in this representation the wave function changes in time only if we take H_1' into account. On the other hand, the dynamical variables satisfy the Heisenberg equations of motion with a Hamiltonian H_0. We shall write the solution of (I. 4) in the form

$$\Phi'(x_0) = S'(x_0)\ \Phi'(-\infty)\ , \tag{I. 6}$$

where $S'(x_0)$ is the so-called scattering operator (scattering matrix, S-matrix). It is clear that

$$i\frac{\partial S'(x_0)}{\partial x_0} = H_1'(x_0)\ S'(x_0)\ . \tag{I. 7}$$

From (I. 6) it follows that the wave functions at $x_0 \to -\infty$ and at $x_0 \to +\infty$ are connected by the relation

$$\Phi'(\infty) = S'(\infty)\ \Phi'(-\infty)\ . \tag{I. 8}$$

The quantity $S'(\infty)$ (usually denoted simply by S') determines thus the probability of all possible transitions in the system, the effective cross-sections, and so on. In the theory of the scattering of particles when H_1' describes the interaction between them and the scattering system it is the natural procedure to assume that the interaction is switched on slowly (adiabatically) and is switched off at the beginning and the end of the process (as $x_0 \to -\infty$ and $x_0 \to +\infty$): $H_1' \sim \exp(-\varepsilon|x_0|)$. In that case $\Phi'(-\infty)$ is the wave function in the Heisenberg representation for the system where $H_1' = 0$. One can say in this context that $S'(x_0)$ is an unitary operator which produces the transition from the Heisenberg to the interaction representation

$$\Phi'(\infty) = S'(\infty)\ \Phi\ , \qquad A'(x_0) = S'(x_0)\ A(x_0)\ S'^{+}(x_0)\ , \tag{I. 9}$$

where A is an arbitrary operator.

From (I. 9) we can, in particular, obtain an expression for any Green function in the interaction representation. Let us for this purpose consider a matrix element of the form

$$M_n = (\Phi_n,\ T\{C_1(x)C_2(x')\}\Phi_n)\ . \tag{I. 10}$$

Using (I. 9) to go over to the interaction representation we get

$$M_n = (\Phi_n',\ T\{C_1'(x)C_2'(x')S'(\infty)\}S'^{-1}(\infty)\Phi_n')\ . \tag{I. 11}$$

In general, $S'^{-1}(\infty)\Phi'$ may be a linear combination of wave functions of very different stationary states. Let us, however, assume that somehow

$$S'^{-1}(\infty)\Phi_n' = a_n\Phi_n'\ , \qquad |a_n| = 1\ , \tag{I. 12}$$

where a_n is a constant. We can then greatly simplify (I. 11) to

$$M_n = a_n(\Phi_n', T\{C_1'(x)C_2'(x')S'(\infty)\}\Phi_n') .$$

By averaging (I. 12) over Φ_n' we easily find a_n:

$$a_n = (\Phi_n', S'(\infty)\Phi_n')^{-1} . \tag{I. 13}$$

If (I. 12) is true for all n, we get, in particular, for any causal Green function

$$K_c(x,x') = i < T\{C_1'(x)C_2'(x')S'\}>' , \tag{I. 14}$$

where the ensemble average is taken with a weight function

$$p_n' = \frac{p_n}{(\Phi_n', S'(\infty)\Phi_n')} .$$

We note, however, that (I. 12) can be satisfied for all n only in some trivial cases. Indeed, this equation indicates that the perturbation H_1' does not cause any real processes to occur in the system, and only leads to the multiplication of the wavefunction by a phase factor a_n. Equation (I. 14) is thus usually not true. An exception is the case $T = 0$ when the averaging in (3. 17) is only over the ground state of the system. This procedure will be indicated by the symbol $<\ldots>_0$. For the ground state wave function (I. 12) is valid: the interaction only leads to a correction of the ground state energy (see (I. 30) below). We have thus for $T = 0$

$$K_c(x,x') = \frac{i}{<S'>_0} < T\{C_1'(x)C_2'(x')S'\}>_0 . \tag{I. 15}$$

We can get formally a closed expression for the scattering matrix by integrating (I. 7) with the initial condition $S'(-\infty) = 1$. We only need remember that $H_1'(x_0)$ and $H_1'(x_0')$ need not commute when $x_0' \neq x_0$. Because of this it is impossible to write the solution of (I. 7) in the following simple exponential form

$$S'(x_0) = \exp\{-i\int_{-\infty}^{x_0} H_1'(t)\,dt\} .$$

One checks easily that the correct equation is

$$S'(x_0) = T\{\exp[-i\int_{-\infty}^{x_0} H_1'(t)\,dt]\} , \tag{I. 16}$$

where the T-product is again defined by (3. 18). The only important point here is that the T-product of operators is ordered in time. The sign of the product which is still open in (3. 18) is here unimportant as the fermion operators occur in the Hamiltonians which interest us only in bilinear (or fourfold) combinations. The choice of sign in (3. 18) is important in another connexion (see the definition of the normal product in the next section of this appendix). We could choose

the initial moment at any time x_0' (not necessarily at $x_0' \to -\infty$). We would then obtain instead of (I. 16)

$$S'(x_0, x_0') = T\{\exp[-i\int_{x_0'}^{x_0} H_1'(t)\,dt]\}\,. \qquad \text{(I. 16a)}$$

If $H_1'(x_0)$ does not contain any time derivatives of field functions, $H_1'(x_0) = -L_1'(x_0)$, where $L_1'(x_0)$ is obtained by the transformation (I. 5) from the corresponding interaction Lagrangian. We get thus

$$S'(x_0) = T\{\exp[i\int_{-\infty}^{x_0} L_1'(t)\,dt]\}\,. \qquad \text{(I. 17)}$$

One can shew (Bogolyubov and Shirkov 1957) that this expression is valid also in the case of an arbitrary (local) interaction Lagrangian. This can be most easily verified by constructing the S-matrix not from the equations of motion but starting directly from the physical requirements of unitarity, covariance, and causality.

We can from (I. 17) obtain a general expression for the probability for any transition in the system (see Berestetskiĭ 1952). As the time occurs in $H_1'(x_0)$ only in an oscillating exponential factor (see (I. 5)) we can verify that the matrix elements of $S'(\infty)$ evaluated in a representation in which H_0' is diagonal are given by

$$(\Phi_n,\, S'(\infty)\Phi_m) = -i\,U_{nm}\int_{-\infty}^{+\infty} e^{i\nu t-\epsilon|t|}\,dt = -2\pi i\,U_{nm}\,\delta(\nu)\,, \qquad \text{(I. 18)}$$

where the U_{nm} are independent of the time, where the factor $-i$ has been separated off for the sake of convenience, and where ν is a quantity which we can easily verify to be simply the difference between the initial and final state energies. The factor $e^{-\epsilon|t|}$ ensures the adiabatic switching on and off of the interaction. The transition probability (per unit time) is

$$w_{nm} = \frac{d}{dx_0}\,|(\Phi_n,\, S'(\infty)\Phi_m)|^2\,. \qquad \text{(I. 19)}$$

As a rule we are interested in the limiting value of w_{nm} as $x_0 \to \infty$. We introduce therefore a quantity

$$s'_{nm}(x_0) = -i\,U_{nm}\int_{-\infty}^{x_0} e^{i\nu t-i\epsilon|t|}\,dt\,,$$

which is the same as the matrix element $(\Phi_n,\, S'\Phi_m)$ only in the limit as $x_0 \to \infty$. If we carry out the integration and then use the definition (I. 19) we find easily

$$w_{nm} = 2\pi\,|U_{nm}|^2\,\delta(\nu)\,. \qquad \text{(I. 20)}$$

One sometimes calls U_{nm} the effective perturbation energy matrix.

b. *Perturbation theory for the S'-matrix; Wick's theorem*

It is still impossible to use (I. 17) immediately for actual calcu-

lations as it contains the ordering symbol T. There are no general prescriptions for getting the operators (I. 17); one uses mostly simply a power series of the exponential, and often afterwards sums its most important terms. We shall consider here this method which is simply a perturbation theory for the S'-matrix, applied to the Hamiltonian (6. 5) with $H_{\text{int}} = 0$. The role of H_1' is played here by the operator of the interaction between the particles and the field:

$$H_1' \equiv H_{\text{pf}}' = - g \int \mathrm{d}^3\vec{x}\; a'^{+}(x)\, \Gamma^{(0)}\, a'(x)\, \Phi'(x)\ , \qquad \text{(I. 21)}$$

and H_0' is the sum of the Hamiltonians of the free particles and of the field. We shall assume that $\Gamma^{(0)}$ does not contain time derivatives; the Lagrangian function L_1' is then given by the right-hand side of (I. 21) with the opposite sign. If we expand the S'-matrix in a series of powers of the coupling constant g, we get from (I. 17)

$$S'(\infty) - 1 = \mathrm{i}\, g \int \mathrm{d}^4x\; a'^{+}(x)\, \Gamma^{(0)}\, a'(x)\, \Phi'(x)$$
$$- \frac{g^2}{2} \int \mathrm{d}^4x\, \mathrm{d}^4x'\; T\, \{a'^{+}(x)\, \Gamma^{(0)}\, a'(x)\, \Phi'(x)\, a'^{+}(x')\, \Gamma^{(0)}\, a'(x')\, \Phi'(x') + \ldots \qquad \text{(I. 22)}$$

In first order in the coupling constant we have only the first term on the right-hand side of (I. 22). It clearly describes processes where boson quanta are emitted and absorbed while at the same time the state of one of the fermions is changed. If we wish to evaluate the transition probability using (I. 20) we must in the usual way write a'^{+} a', and Φ' as linear combinations of the creation and annihilation operators for particles in the states in which we are interested and choose from the sum of products which we obtain in this way the terms of interest. In the given - very simple - case this can easily be done immediately.

The second-order terms on the right-hand side of (I. 22) describe four groups of processes: a) those where the state of the bosons is not changed; b) those where the state of the fermions is not changed; c) those where two bosons are simultaneously emitted (or absorbed); and d) those where one boson is absorbed and another is emitted (this may, in particular, be a boson scattering process). In the last two cases the state of the fermions (that is, of one or two of them) is, of course, also changed.

We could for the evaluation of the corresponding transition probabilities proceed as in the case of the first-order processes, but this would lead here already to very long calculations. The complexity of the calculations increases incredibly rapidly when one goes to the next approximation. It is therefore necessary to formulate some prescriptions which would enable us to write down at once the lowest-order matrix-elements of S' for a particular process. Such a pre-

scription was given by Feynman (1949a,b). This was based mathematically upon Wick's theorem (1950) which we shall now consider.

We first of all introduce the concept of the normal product of operators *. We shall say that the product of elementary (fermion or boson) creation and annihilation operators for particles (quanta) is in normal order, if all creation operators are to the left of all annihilation operators. Let us now have a set of operators $C_1'(x_1)$, $C_2'(x_2), \ldots, C_n'(x_n)$ which are linear combinations of elementary creation and annihilation operators. To obtain the normal product we must explicitly multiply the operators $C_1', \ldots, C_n'$, and then arrange each term in the expression thus obtained in the normal order, assuming that all boson commutators and all fermion anticommutators vanish. In other words, we call a product of operators normal, if independent of the way the operators are written down on paper we let all creation operators act upon the wave function after all annihilation operators have acted upon it. We usually denote a normal product by colons to the right and the left of the operators.

It is clear from the definition that all boson operators (among them $a'(\lambda)$ and $a'^{+}(\lambda)$) under the normal product sign commute and all fermion operators anticommute. This is, in final reckoning, a reflexion of the Pauli principle which is in our definition of the normal product taken into account in the simplest and most natural possible manner.

The principal feature of the normal product of operators is that its vacuum average vanishes. The ground state of the system plays the role of the vacuum when the theory is applied to solid state theory, as we have mentioned several times in the foregoing. When there is no interaction between the particles the ground state of the system is such that one part of the energy levels is completely occupied and the rest completely empty. This makes it possible to introduce in an obvious manner creation and annihilation operators for the excitations, and we must define the normal product in terms of these. The operators a'^{+} and a' occurring in (I. 21) are usually linear combinations of the creation and annihilation operators of the excitations. In order not to complicate the position we shall in the following talk simply about the operators a'^{+} and a' and merely imply those changes which we must introduce when we make this substitution. The ground state of the system is the vacuum for the creation and annihilation operators of the excitations and the average value of the normal product is thus equal to zero in the ground state. (When there are interactions the situation is more complicated, but the interaction is usually included in H_1' while, on the other hand, H_0' describes a system of free particles.) Moreover, if we write the product of operators in the normal form, we see immediately which transitions this product describes. It would therefore be convenient

* Here and henceforth we shall consider only the interaction representation.

for actual calculations to write the T-products which occur in the series for the S'-matrix as a sum of normal products and perhaps some terms which are not operators. This transformation is just what is contained in Wick's theorem. Let us first of all consider a T-product of two operators $T\{C'_1C'_2\}$. By definition we write

$$T\{C'_1C'_2\} = :C'_1C'_2: + \overbrace{C'_1C'_2} \,, \tag{I. 23}$$

where the quantity $\overbrace{C'_1C'_2}$ is defined by this equation and is called the chronological contraction (or simply the contraction) of the operators C'_1 and C'_2. Since the vacuum average of a normal product vanishes, we get from (I. 23)

$$<\overbrace{C'_1C'_2}>_0 = <T\{C'_1C'_2\}>_0 \,. \tag{I. 24}$$

We shall assume now that the contraction $\overbrace{C'_1C'_2}$ is a c-number. (This is the case in the practically most interesting cases.) We can then write (I. 24) simply as

$$\overbrace{C'_1C'_2} = <T\{C'_1C'_2\}>_0 \,. \tag{I. 25}$$

In other words, if the chronological contraction of two operators is a c-number it is apart from a factor i the same as the corresponding causal Green function. This is the reason for the nomenclature "causal": the contractions define those elements of the S'-matrix which describe the causal evolution of the quantum-mechanical system with time. Equation (I. 23) solves thus our problem for the particular case of two operators: we have written $T\{C'_1C'_2\}$ as a sum of a normal product and a term which is not an operator. If we wish to generalise this result to the case of an arbitrary number of operators we must introduce one more concept: that of a normal product with contractions. We emphasise that what follows refers only to the special case where the chronological contraction of any two linear combinations of creation and annihilation operators is a c-number.

Let us consider the product

$$:C'_1(x_1) \ldots \overbrace{C'_j(x_j) \ldots C'_k}(x_k) \ldots C'_n(x_n): \,,$$

where the two operators C'_j and C'_k have undergone a chronological contraction. By definition we put

$$:C'_1(x_1) \ldots \overbrace{C'_j(x_j) \ldots C'_k}(x_k) \ldots C'_n(x_n): = (-1)^{\mathcal{P}} \overbrace{C'_j(x_j)C'_k}(x_k)$$

$$\times :C'_1(x_1) \ldots C'_{j-1}(x_{j-1})C'_{j+1}(x_{j+1}) \ldots C'_{k-1}(x_{k-1})C'_{k+1}(x_{k+1}) \ldots C'_n(x_n): \,. \tag{I. 26}$$

where $\mathcal{P}$ is the parity of the permutation of fermion operators when we change from

$$1, \ldots, j\text{-}1, j, j\text{+}1, \ldots, k\text{-}1, k, k\text{+}1, \ldots, n$$

to $$j, k, 1, \ldots, j\text{-}1, j\text{+}1, \ldots, k\text{-}1, k\text{+}1, \ldots, n\ .$$

Wick's theorem states: the T-product of n linear combinations of creation and annihilation operators is equal to the sum of their normal products with all possible contractions, including the terms without any contractions. A proof of this theorem can be found in any modern text on quantum field theory (for instance, Bogolyubov and Shirkov 1957).

One can easily establish the form of the contractions occurring in Wick's theorem: they are simply the Green functions for the corresponding operators. We note, however, that we must, in fact, have in view here the unperturbed Green functions. One sees, indeed, easily that the contraction of two boson (fermion) operators is a c-numner if, and only if, their commutator (anticommutator) is a c-number. This is true in the interaction representation where the operators satisfy the equations of motion for a free field, but not in the Heisenberg representation. We have thus

$$\overbrace{a'(x)a'^{+}(x')} = -\,\mathrm{i}\,G_c^{(0)}(x, x')\ , \tag{I. 27}$$

$$\overbrace{\Phi'(x)\ \Phi'(x')} = \mathrm{i}\,D_c^{(0)}(x, x')\ , \tag{I. 28}$$

$$\begin{aligned} &\overbrace{a'(x')a'(x)} = \overbrace{a'^{+}(x')a'^{+}(x)} = 0\ , \\ &\overbrace{\Phi'(x)a'(x')} = \overbrace{\Phi'(x')a'^{+}(x)} = 0\ . \end{aligned} \tag{I. 29}$$

One can easily obtain (I. 29) from the law of conservation of the number of particles.

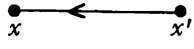
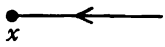
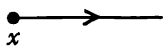
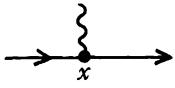
It turns thus, indeed, out to be possible to write the S'-matrix in the normal form. For the following it is convenient to use a special convention about the way we write normal products. It is clear from (I. 21) that in the n-th order of perturbation theory the term without contractions contains the normal product of n pairs of fermion operators

$$:a'^{+}(x_1)a'(x_1)\ \ldots\ a'^{+}(x_n)a'(x_n):\ .$$

In all other terms there will be, by virtue of (I. 29), equal numbers of fermion creation and annihilation operators. We divide them up into pairs in such a way that the terms in each pair correspond to the arguments of the contractions. If we contract, for instance, $a'^{+}(x_i)$ and $a'(x_j)$, we form the pair $a'(x_i)$ and $a'^{+}(x_j)$. We shall arrange the pair terms in such an order that in each pair the a'^{+} is to the left of the a' (the order in which the pairs are taken is clearly immaterial in a normal product). This convention enables us to formulate in the following a rule for the sign of an arbitrary term in the T-product.

c. *Feynman diagrams*

We can in practice write down the terms of the S'-matrix expansion in the normal form most conveniently by a diagrammatic method. It is clear from (I. 21) and (I. 27) to (I. 29) that all terms in the expansion are constructed from three basic "elements": the contractions $iG_c^{(0)}(x, x')$, $iD_c^{(0)}(x, x')$, and the operator product $g\, a'^{+}(x)\, \Gamma^{(0)} a'(x) \Phi'(x)$. We introduce accordingly diagrammatic symbols; they are given in the following table.

Factor	Symbol	Nomenclature
$\overbrace{\Phi'(x)\Phi'(x')}$		Internal boson line
$\overbrace{a'(x)a'^{+}(x')}$		Internal fermion line
$\Phi'(x)$ (in a normal product)		External boson line
$a'(x)$ (in a normal product)		External incoming fermion line
$a'^{+}(x)$ (in a normal product)		External outgoing fermion line
$g\Gamma^{(0)}$ (from the Lagrangian $L_1'(x)$)		Vertex

The terms "internal" and "external" lines are connected with the fact that the first start and end within a diagram, while the latter go to infinity. It is immediately clear from the structure of the S'-matrix expansion that the external lines describe particles which are actually absorbed or emitted during the process considered; on the other hand, the internal lines correspond to virtual processes.

The table gives the connexion between the various factors in the S'-matrix expansion and the diagrammatic symbols.

Let us, in particular, consider some first and second order diagrams which correspond to terms which were written down explicitly in (I. 22). A typical diagram corresponding to first order terms is given in Fig. 1. The presence of two fermion and one boson external line corresponds, as we know, to the emission or absorption of a boson with the concomitant change in the state of one of the fermions.

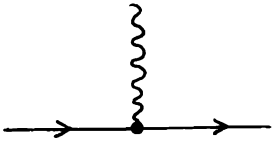


Fig. 1.

Among the diagrams corresponding to the second order terms we note the ones given in Figs. 2 and 3. The first of these describes the influence of virtual electron transitions on the propaga-

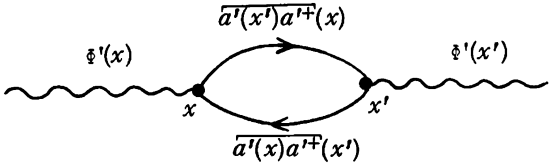


Fig. 2.

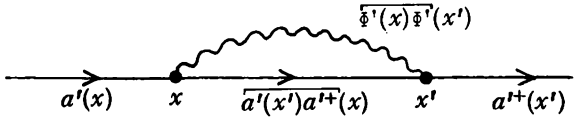


Fig. 3.

tion * of a boson, that is, a "vacuum polarisation" effect; the second describes the influence of the absorption and emission of virtual bosons on the fermion motion ("fermion self energy"), Let us consider one of the third order diagrams (Fig. 4). If we leave out the internal lines we would simply have the diagram of Fig. 1. The internal lines describe the influence of virtual processes on the elementary process of the emission or absorption of a boson: the interaction changes from a point interaction to a non-local one (in the "spreading out" region beyond which the fermion and boson contractions vanish).

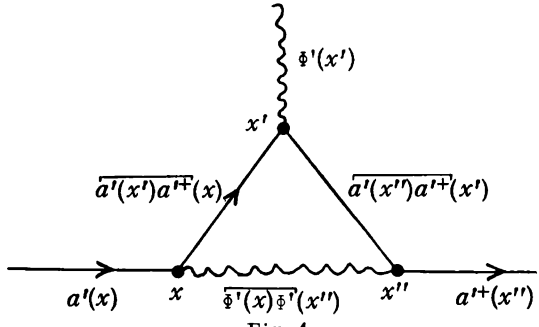


Fig. 4.

The method for bringing the S'-matrix on normal form is now very obvious: for each n-th order term in which we are interested we have n points in each of which three lines meet: two fermion lines (one incoming and one outgoing) and one boson line. The fermion lines will either form closed loops or be external lines ("free ends").

* This is the reason why the Green functions are sometimes called propagators.

Moreover, we must use the rules for getting the correspondence between terms and diagrams, and take the proper signs into account. One verifies easily that each closed fermion loop corresponds to a factor -1.

The procedure outlined here is nothing but the standard quantum-mechanical perturbation theory, put merely in the most convenient form for practical applications. In this connexion the problem arises of finding the sum of the series, or of parts of the series. (This is usually referred to as a summation of diagrams.) It is clear that when we consider a specific effect we must sum only diagrams with the same number and kind of external lines: different orders of perturbation theory differ from one another only through a difference in taking virtual processes into account. In other words, we must first of all draw the simplest diagram describing the process studied in the lowest possible perturbation theory order (such a diagram is called a skeleton). We must then construct in it in all possible ways internal lines (accordingly increasing the number of vertices). The sum of all such diagrams gives, if it converges, the exact value of the S'-matrix element for the process under consideration. We note, in particular one special class of diagrams: the diagrams which do not contain any external lines at all (for instance, Fig. 5) or which contain isolated parts without external lines ("unconnected" diagrams, Fig. 6). They describe "processes" which are not accom-

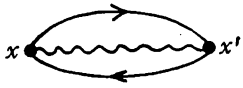


Fig. 5.

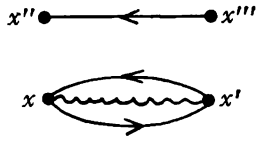


Fig. 6.

panied by any real changes in the system ("vacuum-vacuum" transitions). In quantum field theory the matrix elements of this kind have no meaning and must be eliminated (we shall see presently that they are in fact eliminated automatically in expressions such as (I. 15)); on the other hand, in non-relativistic solid state theory they determine the ground state energy. From our rules it is clear that transitions of this type correspond to a "complete contraction" (not containing any operators at all) of the terms in the S'-matrix expansion. Their sum is thus equal to the vacuum average $\langle S' \rangle_0$. From (I. 16a) we get then easily the formula

$$\langle S'(x_0, x_0') \rangle_0 = \exp\left[- i \, \Delta E (x_0 - x_0') \right] , \qquad \text{(I. 30)}$$

where ΔE is the shift in the ground state energy due to taking the interaction into account. The denominator $\langle S' \rangle_0$ in (I. 15) guarantees at once the elimination of the contributions from the unconnected dia-

grams. (In the many-body problem this causes the spectral representation of the Green functions to contain the differences between the energies of the various states of the system, and not the energies themselves.)

Another important class of diagrams is those with two external lines. One sees easily that the sum of all diagrams with two given external lines is nothing but the corresponding total single-particle Green function *. The sum of all diagrams with one incoming and one outgoing fermion line is the single-fermion Green function (5.2) at absolute zero. That this is so is immediately clear from the definition of the total Green functions as the vacuum averages of the Heisenberg operators. Indeed, the interaction changes at once the operators a'^{+}, a', and Φ' into a^{+}, a, and Φ.

Similarly, the two-particle, three-particle, ... Green functions are also partial sums of the perturbation theory series, corresponding to diagrams with the appropriate number of external lines of the correct type. This fact enables us to sum the diagrams "in stages". We can generalise the cases given by Figs. 2 to 4, we introduce the concepts of self-energy parts, vacuum polarisation parts, and vertex parts. By definition we call a diagram (or part of a diagram) which is connected with its other parts (or the boundaries of the diagram) only through two external fermion lines a self-energy part. It is clear that we obtain it by fitting into the diagram of Fig. 3 all possible internal lines. Similarly we get the vacuum polarisation part by changing the diagram which has only two boson external lines (Fig. 2), and the vertex part by changing the diagram with only two external fermion and one external boson line (Fig. 1). The difference $G_c - G_c^{(0)}$ is thus defined by the sum of all self-energy parts, $D_c - D_c^{(0)}$ by the sum of all vacuum polarisation parts, and $\Gamma - \Gamma^{(0)}$ by the sum of all vertex part diagrams. We introduce, moreover, the concept of irreducible diagrams as those diagrams which do not contain vertex parts, self-energy parts, or vacuum polarisation parts. (An irreducible diagram is, in general, not the same as a skeleton, but may still contain additional internal lines.) The irreducible diagrams obtained from a given skeleton by the addition of different internal lines will be said to belong to the skeleton. It follows from our definitions that, if we wish to evaluate an S'-matrix elements we must

(i) draw the skeleton diagram;

(ii) evaluate the sum of all irreducible diagrams belonging to it;

(iii) replace in that sum the unperturbed Green functions $G_c^{(0)}$, $D_c^{(0)}$, and vertex part $\Gamma^{(0)}$ by the exact G_c, D_c, and Γ. We must then substitute in the external lines the "renormalised" fermion and boson

* We remind ourselves that the Green functions are here defined as vacuum (ground state) averages.

energies (that is, those evaluated taking the interaction fully into account). This procedure we shall call the Dyson rules as he was the first to give them (Dyson 1949) in the framework of quantum electrodynamics.

In quantum field theoretical problems the "renormalised" energies - with an appropriate definition of the T-products when the arguments coincide - are the same as the "initial" ("bare") energies (Bogolyubov and Shirkov 1957), and one therefore sometimes states that one needs not make any changes in the external lines. In solid state theory, however, the difference between the "renormalised" and the "bare" energies describes real physical effects (for instance, the excitation of plasma oscillations) and the substitution mentioned a moment ago is necessary. One verifies this very easily by evaluating the S'-matrix elements through using Fourier transforms with respect to the time and taking into account the connexion between the excitation spectrum and the poles of the Green functions (sections 4, 5, and 16). When there are several kinds of excitations present there will appear the same number of kinds of external lines (corresponding to the different kinds of poles of Green functions).

We note that the definition of the irreducible diagrams given above is not an "absolute" one, but depends on with respect of which Green function it is made. In the general case a diagram is called an irreducible one if it does not contain elements the sum of which gives Green functions which are in the case under consideration taken explicitly into account (apart from the skeleton elements, of course). If we included, for instance, in our considerations apart from the above mentioned Green functions also the two-fermion Green function, we should consider diagrams which do not contain "four-poles" - that is, parts which are joined to the rest of the diagrams only by two pairs of fermion lines - also to be irreducible. We should reformulate the Dyson rules accordingly, adding to them the requirement of replacing $G_{2c}^{(0)}$ by G_{2c}.

Of course, the Dyson rules by themselves - or any other similar rule - do not solve the problem of evaluating the S'-matrix, but only divide it into several stages - and this may be very useful for purely calculational purposes. In all cases, however, one must eyaluate several partial sums from the perturbation theory series and this is usually reduced to the solution of some integral equations. The simplifications which one then must take are based upon justified estimates of the contributions from different diagrams. If the coupling constant is sufficiently small it is sometimes, indeed, possible to split off a class of diagrams which give the main contribution to some specific scattering matrix elements. If we discard all other corrections we proceed to the so-called method of the summation of the important diagrams which (at $T = 0$) is equivalent to the improved perturbation theory given in section 11.

The Dyson equations for the Green functions can (at the absolute zero) themselves be diagrammatically represented. To do this we put shaded circles on all internal lines which may still contain all possible "insertions". If we then use our rules we can depict (10. 1) and (10. 2) as is done in Fig. 7. The mass and polarisation operators which are given by (10. 4) and (10. 5) are depicted in Fig. 8.

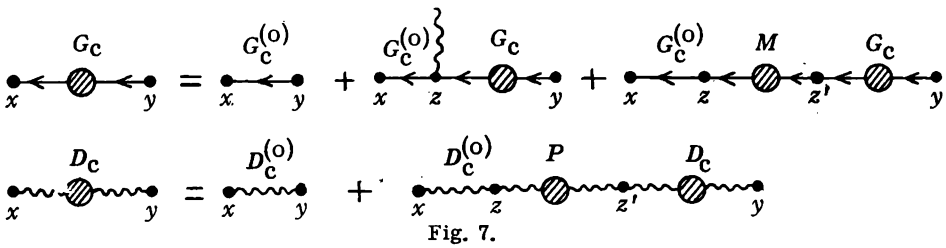


Fig. 7.

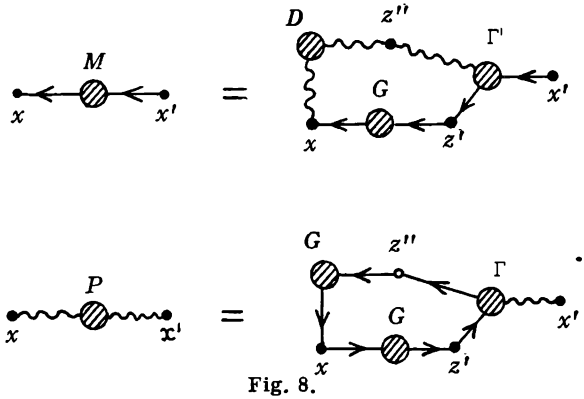


Fig. 8.

We wish to make two final remarks.

First of all, all discussions of summations of diagrams have a purely formal character as they are based upon well-defined assumptions about the analytical properties of the functions we are looking for. In particular, one assumes implicitly that the perturbation theory series converges for $g = 0$. In actual cases, however, this assumption may well turn out not to be justified. In quantum electrodynamics, for instance, the perturbation theory series is, apparently an asymptotic one (Bogolyubov and Shirkov 1957). The method of summing the "important diagrams" may thus no longer be unique (see Redmond 1958, Bogolyubov, Logunov, and Shirkov 1959).

Secondly, the diagrammatic method in the form described here is connected with the averaging over the ground state of the system ($T = 0$). Its generalisation to the case of temperature-dependent Green functions requires well-known modifications; we do not wish to discuss these here.

d. *Commutation rules when the two time arguments are the same*

The Lagrangian of the free electromagnetic field is of the form (see, for instance, Bogolyubov and Shirkov 1957)

$$L_0(x) = -\tfrac{1}{2} \sum_\beta : g^{\beta\beta} \{ \frac{1}{c_0^2} \left(\frac{\partial A_\beta(x)}{\partial x_0}\right)^2 - \sum_{i=1,2,3} \left(\frac{\partial A_\beta(x)}{\partial x_i}\right)^2 \} : . \quad \text{(I. 31)}$$

The components of the four-potential $A_\beta(x)$ play here the role of the generalised coordinates. The generalised momenta are thus

$$\mathcal{P}^\beta(x) = \frac{\partial L_0}{\partial \frac{\partial A_\beta}{\partial x_0}} = -\frac{1}{c_0^2} g^{\beta\gamma} \frac{\partial A_\gamma(x)}{\partial x_0} . \quad \text{(I. 32)}$$

The canonical commutation rules are thus

$$[A_\beta(\vec{x}, x_0),\ A_\gamma(\vec{x}', x_0)]_- = 0 , \quad \text{(I. 33)}$$

$$[\frac{\partial A_\beta(\vec{x}, x_0)}{\partial x_0} ,\ A_\gamma(\vec{x}', x_0)]_- = \mathrm{i}\, c_0^2\, g_{\beta\gamma}\, \delta(\vec{x}-\vec{x}') . \quad \text{(I. 34)}$$

By differentiating (I. 33) with respect to x_i we get

$$[\frac{\partial A_\beta(\vec{x}, x_0)}{\partial x_i} ,\ A_\gamma(\vec{x}', x_0)]_- = 0 . \quad \text{(I. 35)}$$

e. *A uniform dielectric and magnetic medium*

We shall consider an electromagnetic field for the case where there are no free charges in a spatially uniform medium characterised by real scalar dielectric and magnetic susceptibilities ϵ and μ.

It is well known that one can then write the classical Maxwell equations in the form *

$$\vec{B} = \mathrm{curl}\, \vec{A} , \quad \vec{E} = -\frac{1}{c_0} \frac{\partial \vec{A}}{\partial t} + \vec{\nabla} A_0 , \quad \text{(I. 36)}$$

$$\frac{\epsilon\mu}{c_0^2} \frac{\partial^2 A_\beta}{\partial t^2} - \nabla^2 A_\beta = 0 , \quad \text{(I. 37)}$$

$$\frac{\epsilon\mu}{c_0} \frac{\partial A_0}{\partial t} - \mathrm{div}\, \vec{A} = 0 , \quad \text{(I. 38)}$$

$$\vec{B} = \mu \vec{H} , \quad \vec{D} = \epsilon \vec{E} . \quad \text{(I. 39)}$$

The two equations

$$\mathrm{div}\, \vec{B} = 0 , \quad \mathrm{curl}\, \vec{E} = -\frac{1}{c_0} \frac{\partial \vec{B}}{\partial t}$$

* We consider only a frame of reference fixed in the medium. A formulation which is covariant under a Lorentz transformation can, for instance, be found in papers by Jauch and Watson (1948a, b; 1949) and by Ryazanov (1957).

are satisfied automatically by virtue of (I. 36), and the other pair

$$\operatorname{div} \vec{D} = 0 , \qquad \operatorname{curl} \vec{H} = \frac{1}{c_0} \frac{\partial \vec{D}}{\partial t}$$

is equivalent to (I. 36) and (I. 37), if we take (I. 49) and the Lorentz condition (I. 38) into account.

One verifies easily that one can obtain (I. 37) immediately from the Lagrangian

$$\begin{aligned} L(x) = -\tfrac{1}{2} \sum_{\beta} g^{\beta\beta} \Big\{ \frac{1}{c_0^2} \Big(\frac{\partial A_\beta}{\partial x_0}\Big)^2 - \sum_{i=1,2,3} \Big(\frac{\partial A_\beta}{\partial x_i}\Big)^2 \Big\} \\ + \frac{n^2 - 1}{2} \sum_{i=1,2,3} \Big(\frac{\partial A_0}{\partial x_i} - \frac{1}{c_0} \frac{\partial A_i}{\partial x_0}\Big)^2 - \frac{(n^2-1)^2}{2\, c_0^2} \Big(\frac{\partial A_0}{\partial x_0}\Big)^2 \\ - (n^2 - 1) \frac{1}{c_0} \frac{\partial A_0}{\partial x_0} \Big\{ \frac{1}{c_0} \frac{\partial A_0}{\partial x_0} - \sum_{i=1,2,3} \frac{\partial A_i}{\partial x_i} \Big\} . \end{aligned} \tag{I. 40}$$

Here $n^2 = \varepsilon\mu$. Equation (I. 40) is a direct generalisation of (I. 31) for the case of the dielectric and magnetic medium considered here. When we quantise this problem, we must consider all products in (I. 40) to be normal products and replace (I. 38) by a similar condition imposed upon the allowed wave functions of the system or - which amounts to the same - upon the average of the operators A_β. Completely analogously to (I. 32) we find for the generalised momenta

$$\mathcal{P}^0(x) = -\frac{n^4}{c_0^2} \frac{\partial A_0}{\partial x_0} + \frac{n^2 - 1}{c_0} \sum_i \frac{\partial A_i}{\partial x_i} , \tag{I. 41}$$

$$\mathcal{P}^i(x) = \frac{n^2}{c_0^2} \frac{\partial A_i}{\partial x_0} - \frac{n^2 - 1}{c_0} \frac{\partial A_0}{\partial x_i} . \tag{I. 42}$$

The commutation relations (I. 33) and (I. 35) remain valid and instead of (I. 34) we get

$$\Big[\frac{\partial A_\beta(\vec{x}, x_0)}{\partial x_0} , A_\gamma(\vec{x}', x_0)\Big]_- = i \frac{c_0^2}{n^2} g_{\beta\gamma} \Big(\delta_{\beta i} + \frac{\delta_{\beta 0}}{n^2}\Big) \delta(\vec{x} - \vec{x}') . \tag{I. 43}$$

We do not sum here over β. One can also easily find the appropriate four-dimensional commutation relations (Ryazanov 1957) but we do not need them here.

By considering (I. 36) to (I. 43) one verifies easily that we can completely eliminate ε and μ from the field equations, if we

(i) everywhere replace the velocity of light in vacuo c_0 by the velocity of light in the medium, $c = c_0/\sqrt{\varepsilon\mu}$;

(ii) replace the actual components of the potential (and the field) by the "renormalised" quantities

$$A_{i,r} = A_i , \qquad A_{0,r} = \sqrt{\varepsilon\mu}\, A_0 , \qquad \vec{B}_r = \vec{B} , \qquad \vec{E}_r = \sqrt{\varepsilon\mu}\, \vec{E} ; \tag{I. 44}$$

and (iii) replace the true field energy W by the "renormalised" quantity

$$W_r = \mu W \ . \tag{I. 45}$$

We have, for instance, for the energy density in the electromagnetic field in vacuo the expression $\frac{1}{2}(\vec{E}^2+\vec{B}^2)$; if we consider this quantity to be W_r, we get for the energy density in the dielectric from (I. 44) and (I. 45)

$$\frac{\varepsilon\mu\,\vec{E}^2 + \vec{B}^2}{2\mu} = \frac{\varepsilon\,\vec{E}^2 + \mu\,\vec{H}^2}{2} \ ,$$

as should be the case. The renormalised fields $\vec{E}$ and $\vec{B}$ satisfy then the usual Maxwell equations in vacuo (with c replaced by c_0).

When there are currents and free charges present we can also formally eliminate ε and μ from the Maxwell equations if we introduce apart from the renormalised potential also renormalised charges and currents:

$$e_r = \sqrt{\frac{\mu}{\varepsilon}}\, e \ , \qquad J_r = \sqrt{\frac{\mu}{\varepsilon}}\, J \ . \tag{I. 46}$$

To see this one just writes down (I. 37) with the appropriate right hand sides.

When the dielectric and magnetic susceptibilities shew dispersion (I. 44) to (I. 46) remain valid for the various Fourier components.

Apart from in Chapter VII we have used in the main body of this book everywhere renormalised quantities, without writing the index "r" down explicitly.

f. *Interactions through a field and direct interactions*

Equations (I. 18) and (I. 22) together with the Dyson rules enable us, in particular, to consider the problem of the connexion between the interaction through a field and the direct pair-interaction, and to elucidate when these two representations are equivalent.

Let us consider a system of fermions interacting with a quantised field according to (I. 22). We saw in subsection b) of this appendix that the scattering matrix in second order contains elements describing the change of fermion states without a concomitant change in the states of the boson field. Physically these elements correspond, for instance, to fermion-fermion scattering processes; the boson field only serves then to transfer the interaction. Such processes may occur also when there are no boson quanta present (in the "boson vacuum"). We obtain the corresponding S'-matrix elements by evaluating the average (I. 22) for states where there are no bosons ("average over the boson vacuum"). We shall indicate this procedure by the symbol $<\ldots>_{B,0}$ and give S' an index 2, indicating that we are only considering second order terms. From (I. 22) we have

$$\langle S_2(\infty)\rangle_{B,0} = -\frac{g^2}{2}\int d^4x\, d^4x'\, T\,\{a'^+(x)\,\Gamma^{(0)}\,a'(x)\,a'^+(x')\times\Gamma^{(0)}\,a'(x')\}\,i\,D_c^{(0,0)}(x,x')\,, \tag{I. 47}$$

where

$$D_c^{(0,0)}(x,x') = -i\langle\Phi'(x)\Phi'(x')\rangle_{B,0}\,.$$

The superscript (o,o) (and not simply "o") is used here to indicate that the average is taken here over a boson vacuum in a system with two particles (and not over a state of a many-body system).

Processes corresponding to an interaction between fermions are described by the matrix elements of (I. 47) which connect two states of the system with two particles in them (we shall indicate this by $\langle S'(\infty)\rangle_{B,0,F,2}$). We shall assume that initially and finally the particles are in stationary states characterised by some quantum numbers λ. In accordance with this we write the a'^+ and a' in (I. 47) in the λ-representation:

$$\begin{aligned} a'(x) &= \sum_\lambda \psi_\lambda(\vec{x})\, e^{-iW(\lambda)x_0}\, a'(\lambda)\,,\\ a'^+(x) &= \sum_\lambda \psi_\lambda^+(\vec{x})\, e^{iW(\lambda)x_0}\, a'^+(\lambda)\,. \end{aligned} \tag{I. 48}$$

Here the $\psi_\lambda(\vec{x})$ are, as always, the eigenfunctions of the operator corresponding to the dynamical variable λ (they may, for instance, be the eigenfunctions of the "single-particle" Hamiltonian), $W(\lambda)$ the corresponding eigenvalues, and $a'^+(\lambda)$ and $a'(\lambda)$ the operators which create and annihilate particles in the state λ. Let the values of λ in the initial and final states of our two particles be λ_1, λ_2 and λ_3, λ_4. We can now easily evaluate the matrix elements of the T-product in (I. 47). We shall then obtain two pairs of terms, and the terms occurring in a given pair give the same result after integration (if we take the symmetry of $D_c^{(0,0)}$ into account). We have thus for $\langle S'_2(\infty)\rangle_{Bo,F2}$ a sum of two terms

$$\langle S'_2(\infty)\rangle_{Bo,F2} = S'_{12,34} - S'_{12,43}\,, \tag{I. 49}$$

where

$$S'_{12,34} = -\,i\,g^2\int d^4x\, d^4x'\, D_c^{(0,0)}(x,x')\,\psi_4^+(\vec{x}')\,\Gamma^{(0)}\,\psi_2(\vec{x}')\,\psi_3^+(\vec{x})\,\Gamma^{(0)}\,\psi_1(\vec{x})$$
$$\exp\{i\,[W(\lambda_4) - W(\lambda_2)]\,x'_0 + i\,[W(\lambda_3) - W(\lambda_1)]\,x_0\}\,, \tag{I. 50}$$

while $S'_{12,43}$ is obtained from (I. 50) by interchanging 3 and 4 (this term is called the exchange term compared to the first one). The minus-sign in (I. 49) is connected with the fact that we are dealing with fermions; if we were dealing with bosons we would have (I. 49) but with a plus-sign. We shall expand $D_c^{(0,0)}(x,x')$ in a Fourier integral with respect to the time

$$D_c^{(o,o)}(x, x') = \int_{-\infty}^{+\infty} d\omega \, e^{-i\omega(x_o - x'_o)} \, D_c^{(o,o)}(\vec{x}, \vec{x}'; \omega) \, , \qquad (I.51)$$

and we introduce short-hand notations such as

$$W(\lambda_4) - W(\lambda_2) = \omega_{42} \, . \qquad (I.52)$$

We then get from (I. 50)

$$S'_{12,34} = - i g^2 (2\pi)^2 \, \delta(\omega_{42}+\omega_{31}) \int d^3\vec{x} \, d^3\vec{x}' \, \psi_4^+(\vec{x}') \, \Gamma^{(o)} \, \psi_2(\vec{x}')$$

$$\times D_c^{(o,o)}(\vec{x}, \vec{x}'; \frac{\omega_{42}-\omega_{31}}{2}) \, \psi_3^+(\vec{x}) \, \Gamma^{(o)} \, \psi_1(\vec{x}) \, . \qquad (I.53)$$

From (I. 52) we see that

$$\omega_{42} + \omega_{31} = \omega_{32} + \omega_{41} = W(\lambda_4) + W(\lambda_3) - W(\lambda_2) - W(\lambda_1) \, .$$

We see thus that the δ-function in (I. 53) expresses simply, as we should have expected, the law of conservation of energy during scattering. From (I. 18) we find now the matrix of the effective perturbation theory

$$U = U_{12,34} - U_{12,43} \, , \qquad (I.54)$$

$$U_{12,34} = 2\pi g^2 \int d^3\vec{x} \, d^3\vec{x}' \, \psi_4^+(\vec{x}') \, \Gamma^{(o)} \, \psi_2(\vec{x}')$$

$$\times D_c^{(o,o)}(\vec{x}, \vec{x}'; \frac{\omega_{42}-\omega_{31}}{2}) \, \psi_3^+(\vec{x}) \, \Gamma^{(o)} \, \psi_1(\vec{x}) \, . \qquad (I.55)$$

The quantity $U_{12,43}$ is obtained by interchanging 3 and 4.

Equation (I. 55) is similar to the usual quantum mechanical expression for the average energy of a pair interaction (if we take for the interaction energy the quantity $2\pi g^2 D_c^{(o,o)}$). We must, however, point to the following important fact: the function $D_c^{(o,o)}(\vec{x}, \vec{x}'; \frac{1}{2}(\omega_{42}-\omega_{31})$ depends on the states between which the transition takes place. The resemblance between (I. 55) and the average interaction energy is a purely superficial one, and it is in general impossible to talk about a potential energy for the direct interaction between the particles. An exception is the case when the function $D_c^{(o,o)}(\vec{x}, \vec{x}'; \omega)$ is practically independent of ω (or, what comes to the same, if we may neglect the "transition frequencies" ω_{42} and ω_{31} as compared to some constant frequency occurring in $D_c^{(o,o)}$). In that case, the right-hand side of (I. 55) is, indeed, the average energy of the binary interaction, which is described by the operator

$$U_o = 2\pi g^2 \, \Gamma^{(o)} \, D_c^{(o,o)}(\vec{x}, \vec{x}') \, \Gamma^{(o)} \, , \qquad (I.56)$$

where the index "o" of U indicates that (I. 56) is the result of taking only the first non-vanishing approximation. It is clear from (I. 51) that the dependence of $D_c^{(o,o)}(x, x')$ on its time arguments has then a

delta-function character: $D_c^{(0,0)}(x,x') \sim \delta(x_0 - x_0')$. In other words, in the case considered the interaction is instantaneous and there is no retardation.

It thus turns out to be possible, if we neglect retardation and work in the second order approximation in the coupling constant g, to introduce an operator (I. 56) of the potential energy for the direct interaction between the particles. This is true both for fermions and for bosons. In the latter case we need only change the sign in (I. 54) from a minus to a plus. It follows from (I. 20) that the probabilities for all processes which do not involve a change in the state of the field are determined by the matrix elements of this operator. This means that as long as we are interested only in such processes we can completely "forget" the existence of the field and replace the exact Hamiltonian (I. 21) by a Hamiltonian involving binary interactions such as (6. 8a).

We can change from the second ("first non-vanishing") approximation to an exact expression for the S'-matrix which takes into account all approximations by using Dyson's rules. There may then occur additional complications which may restrict the applicability of the standard formulation of an interaction potential energy even more. To elucidate the nature of these complications it is sufficient to consider merely the approximation where we have only replaced $D_c^{(0,0)}$ and $\Gamma^{(0)}$ by the corresponding exact expressions. In that case we get for the S'-matrix elements in which we are interested (compare (I. 53))

$$S'_{12,34} = -\,i\,g^2 \int D_c(z,z')\,\psi_4^+(\vec{y})\,\Gamma(y,y';z')\,\psi_2(\vec{y}')\,\psi_3^+(\vec{x})\,\Gamma(x,x';z)\,\psi_1(x') \times \exp\left[i\,W(\lambda_4)y_0 - i\,W(\lambda_2)y_0' + i\,W(\lambda_3)x_0 - i\,W(\lambda_1)x_0'\right] \times d^4z\,d^4z'\,d^4y\,d^4y'\,d^4x\,d^4x' . \tag{I. 57}$$

If we put

$$D_c(z,z') = \int d\omega\, e^{-i\omega(z_0 - z_0')}\, D_c(\vec{z},\vec{z}';\omega) ,$$

$$\Gamma(x,x';z) = \frac{1}{(2\pi)^2} \int d\omega'\,d\omega''\, e^{-i\omega'(x_0 - z_0) - i\omega''(x_0' - z_0)}\, \Gamma(\vec{x},\vec{x}';\vec{z};\omega',\omega'') , \tag{I. 58}$$

we get

$$S_{12,34} = -\,i\,g^2 \int d^3\vec{z}\,d^3\vec{z}'\,d^3\vec{x}\,d^3\vec{x}'\,d^3\vec{y}\,d^3\vec{y}'\,(2\pi)^2\,\delta(\omega_{42}+\omega_{31})\,\psi_4^+(\vec{y}) \times \Gamma(\vec{y},\vec{y}';\vec{z}';W_4,W_2)\,\psi_2(\vec{y}')\,D_c(\vec{z},\vec{z}';\tfrac{\omega_{42}-\omega_{31}}{2})\,\psi_3^+(\vec{x}) \times \Gamma(\vec{x},\vec{x}';\vec{z};W_3,W_1)\,\psi_1(\vec{x}') , \tag{I. 59}$$

and thus

$$U_{12,34} = 2\pi g^2 \int d^3\vec{z}\; d^3\vec{z}'\; d^3\vec{x}\; d^3\vec{x}'\; d^3\vec{y}\; d^3\vec{y}'\; \psi_4^+(\vec{y})$$
$$\times\, \Gamma(\vec{y},\vec{y}';\vec{z}';W_4,W_2)\, \psi_2(\vec{y}')\, D_c(\vec{z},\vec{z}';\tfrac{\omega_{42}-\omega_{31}}{2})$$
$$\times\, \psi_3^+(\vec{x})\, \Gamma(\vec{x},\vec{x}';\vec{z};W_3,W_1)\, \psi_1(\vec{x}')\,. \qquad (I.60)$$

As in the simplest case (I. 55) the right-hand side of (I. 60) reminds us of the expression for the matrix element of an operator; we can, however, also in the present case introduce such an "interaction energy operator" in actual cases only if we neglect retardation. Moreover, the neglect of retardation is here connected with even larger limitations as it is necessary that we can neglect the frequency dependence of the Fourier transforms of both the total Green function D_c and of the vertex part Γ. As a rule this can be done only approximately, even if the Fourier transform of the "unperturbed" function $D_c^{(o,o)}$ were independent of the frequency.

If, finally, all these approximations are possible, then we do still not obtain the simple, usual "classical" formula (I. 56). Indeed, we get from (I. 60) for the operator of the energy of the direct interaction between the particles (provided we can introduce it) the expression

$$U(\vec{y},\vec{x};\vec{y}',\vec{x}') = 2\pi g^2 \int d^3\vec{z}\; d^3\vec{z}'\; \Gamma(\vec{y},\vec{y}';\vec{z}')\, D_c(\vec{z},\vec{z}')\, \Gamma(\vec{x},\vec{x}';\vec{z})\,. \qquad (I.61)$$

This quantity depends on two pairs of points (that is, on three vectors; for instance, on $\vec{x}$-$\vec{x}'$, $\vec{x}$-$\vec{y}$, and $\vec{y}$-$\vec{y}'$) instead of on one pair. The corresponding binary direct interaction Hamiltonian is thus of the general form (6. 8) without any of the simplifications which led to (6. 8a).

The replacing of the interaction through a field by a direct pair interaction is thus possible only under well-defined limiting conditions and for a well-defined class of problems. On the other hand, the inverse replacement, namely the description of a direct interaction by an interaction through a field, is clearly always possible, provided U is finite *: we need only determine the Fourier transform of $D_c(\vec{x},\vec{x}';\omega)$ from (I. 61); the vertex part can in this case always be assumed to have a delta-function character. In that case we get thus in the coordinate representation

$$g^2\, D_c(x,x') = \delta(x_o - x_o')\, U(\vec{x}-\vec{x}')\,. \qquad (I.62)$$

To avoid misunderstandings we note that we understand here by the exact Green function D_c the expression which is exact inasfar as we consider the interaction between two particles and virtual quanta in

* This excludes singular potentials such as the hard-sphere potential.

the field. Effects connected with a collective interaction between particles, such as screening, are here, of course, not taken into account: they arise only in a many-body system. From the many-body theory point of view (I. 62) is $D_c^{(0)}$, and this is the reason why we denoted the "unperturbed" Green function in the foregoing by $D_c^{(0,0)}$.

Appendix II

PAULI OPERATORS *

Operators $b(\lambda)$ and $b^+(\lambda)$ which satisfy the commutation relations

$$b(\lambda')b^+(\lambda) - b^+(\lambda)b(\lambda') = 0\ ,\quad b(\lambda)b(\lambda') - b(\lambda')b(\lambda) = 0\ ,\quad \lambda' \neq \lambda\ , \tag{II. 1}$$

$$b(\lambda)b^+(\lambda) + b^+(\lambda)b(\lambda) = 1\ ,\quad b(\lambda)b(\lambda) + b(\lambda)b(\lambda) = 0\ , \tag{II. 2}$$

are called Pauli operators.

One notes immediately that (II. 1) and (II. 2) are a combination of boson (for $\lambda' \neq \lambda$) and fermion (for $\lambda' = \lambda$) commutation relations.

The Pauli operators are closely connected with spin operators. Indeed, let us put $\lambda = f$ (f numbers the lattice sites) and let us introduce the quantities

$$S_1(f) = -\,[b(f) + b^+(f)]\ ,\qquad S_2(f) = \mathrm{i}\,[b(f) - b^+(f)]\ ,$$
$$S_3(f) = 1 - 2\mathfrak{n}(f)\ , \tag{II. 3}$$

where $\mathfrak{n}(f) = b^+(f)b(f)$, or,

$$S_1(f) = b(f) + b^+(f)\ ,\qquad S_2(f) = \mathrm{i}\,[b^+(f) - b(f)]\ ,$$
$$S_3(f) = 1 - 2\mathfrak{n}(f)\ . \tag{II. 4}$$

From (II. 1) and (II. 2) we then easily verify that the S_i satisfy the commutation relations for the electron spin components (apart from factors $\hbar/2$). The general representation of the $S_i(f)$ operators in terms of the $b^+(f)$ and $b(f)$ is of the form

$$S_i(f) = \sigma_i(f)\,[1 - 2\mathfrak{n}(f)] + A_i(f)b(f) + A_i^+(f)b^+(f)\ , \tag{II. 5}$$

where the $\sigma_i(f)$ are the components of a classical unit vector and where

$$A_1(f) = -\,e^{\mathrm{i}\gamma f}\,\frac{1 + \sigma_3(f)}{2} + e^{-\mathrm{i}\gamma f}\,\frac{1 - \sigma_3(f)}{2}\ ,$$

$$A_2(f) = \mathrm{i}\,[e^{\mathrm{i}\gamma f}\,\frac{1 + \sigma_3(f)}{2} + e^{-\mathrm{i}\gamma f}\,\frac{1 - \sigma_3(f)}{2}]\ , \tag{II. 6}$$

$$A_3(f) = \sqrt{1 - \sigma_3^2(f)}\ ,\qquad \gamma_f = \arctan\frac{\sigma_2(f)}{\sigma_1(f)}\ .$$

* Tyablikov 1956, Bogolyubov 1958b.

Comparing (II. 3) and (II. 5) we get the formulae for a canonical transformation for the Pauli operators. For practical purposes it is sufficient to consider the particular case when $\sigma_2(f) = 0$. We get then

$$\begin{aligned}
\beta(f) &= -u(f)v(f)\,[1 - 2\mathfrak{n}(f)] + u^2(f)b(f) - v^2(f)b^+(f)\,, \\
\beta^+(f) &= -u(f)v(f)\,[1 - 2\mathfrak{n}(f)] + u^2(f)b^+(f) - v^2(f)b(f)\,, \qquad \text{(II. 7)} \\
\beta^+(f)\beta(f) &= v^2(f) + [u^2(f) - v^2(f)]\,\mathfrak{n}(f) - u(f)v(f)\,[b(f) + b^+(f)]\,,
\end{aligned}$$

where the $\beta(f)$ and $\beta^+(f)$ are the new Pauli operators. The functions $u(f)$ and $v(f)$ are here real functions, connected by the relations

$$u^2(f) + v^2(f) = 1\,, \qquad u^2(f) = \frac{1 + \sigma_3(f)}{2}\,, \qquad v^2(f) = \frac{1 - \sigma_3(f)}{2}\,. \qquad \text{(II. 8)}$$

It follows, in particular, from (II. 7) that a linear transformation is not a canonical one for the Pauli operators.

Appendix III

THE CAUSAL GREEN FUNCTION FOR A FREE ELECTROMAGNETIC FIELD

We shall call the electromagnetic field in a uniform dielectric medium which is characterised by scalar dielectric and magnetic susceptibilities ϵ and μ a free one, as was done in the main text; the light velocity c is the velocity in such a medium. The causal Green function is by definition

$$D^{(o)}_{c,\beta\gamma}(x, x') = -\,i\,\langle T\,\{A_\beta(x)\,A_\gamma(x')\}\rangle\,. \qquad \text{(III. 1)}$$

The averaging is here over states of the free electromagnetic field. In particular, this is at $T = 0$ an average over the ground state of the field: the free photon vacuum. We shall restrict ourselves in the following to that case. As the $A_\beta(x)$ satisfy the d'Alembert equation one checks easily that (III. 1) is a solution of the equation

$$\Box\, D^{(o)}_{c,\beta\gamma}(x, x') = -\frac{i}{c^2}\,\delta(x_o - x'_o)\,\langle\left[\frac{\partial A_\beta(x)}{\partial x_o}\,,\, A_\gamma(x')\right]_-\rangle\,. \qquad \text{(III. 2)}$$

From (I. 54) it follows that the right-hand side of (III. 2) is equal to $g_{\beta\gamma}\delta(x-x')$. We write (III. 1) in the spectral form such as (3. 19) or (3. 20) to formulate the boundary conditions which single out the solution we want:

$$D^{(o)}_{c,\beta\gamma}(x, x') = \int_{-\infty}^{+\infty} dE\, e^{-iE(x_o - x'_o)}\, D^{(o)}_{c,\beta\gamma}(\vec{x}, \vec{x}'; E)\,, \qquad \text{(III. 3)}$$

$$D^{(o)}_{c,\beta\gamma}(\vec{x}, \vec{x}'; E) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} dE'\,\left\{\frac{J_1(\vec{x}, \vec{x}'; E')}{E' - E - i\epsilon} - \frac{J_2(\vec{x}, \vec{x}'; E')}{E' - E + i\epsilon}\right\}\,, \qquad \text{(III. 4)}$$

where

$$J_1(\vec{x}, \vec{x}'; E') = \sum_n (\Phi^{(o)}_o, A_\beta(\vec{x}, 0)\Phi^{(o)}_n)(\Phi^{(o)}_n, A_\gamma(\vec{x}', 0)\Phi^{(o)}_o)\,\delta(E' - E_n)\,, \qquad \text{(III. 5)}$$

$$J_2(\vec{x}, \vec{x}'; E') = \sum_n (\Phi^{(o)}_o, A_\gamma(\vec{x}', 0)\Phi^{(o)}_n)(\Phi^{(o)}_n, A_\beta(\vec{x}, 0)\Phi^{(o)}_o)\,\delta(E' + E_n)\,. \qquad \text{(III. 6)}$$

We have here already taken into consideration that the average is over the free photon vacuum with wave function $\Phi^{(o)}_o$ and energy which can be taken to be equal to zero. We have clearly $E_n \geq 0$, that is, J_1 contains only positive, and J_2 only negative frequencies. Substituting (III. 4) into (III. 3) and integrating over E, we see that

$D_c^{(0)}(x, x')$ contains only positive frequencies, if $x_0' < x_0$, and only negative ones, if $x_0' > x_0$. This is the required boundary condition (Feynman condition). If we write $D_c^{(0)}(x, x')$ as a four-dimensional Fourier integral and use (III. 2) together with the Feynman condition we get (5. 35) and (5. 38).

We note that one can also use a spectral representation such as (III. 4) (but for $T \neq 0$) to find easily $D_c^{(0)}(x, x')$ for the general case when we take thermal radiation into consideration.

Appendix IV

THE SPECTRAL REPRESENTATIONS FOR MANY-TIME GREEN FUNCTIONS *

Let us consider triple products such as

$$K(x,x',x'') = \langle C_1(x)C_2(x')C_3(x'')\rangle . \qquad \text{(IV. 1)}$$

In thermodynamic equilibrium this quantity depends only on the differences between the time arguments. Let us write $x_0 - x_0' = t$, $x_0' - x_0'' = t'$. Proceeding as in section 2 we get

$$K(x,x',x'') = \sum_{n,m,l} p_n(\Phi_n, C_1(x)\Phi_m)(\Phi_m, C_2(x')\Phi_l)(\Phi_l, C_3(x'')\Phi_n)$$

$$= \int_{-\infty}^{+\infty} dE\, dE'\, e^{-iEt - iE't'}\, J(\lambda, \lambda', \lambda''; E, E') , \qquad \text{(IV. 2)}$$

where the spectral function J is given by the equation

$$J(\lambda, \lambda', \lambda''; E, E') = \sum_{n,m,l} p_n(\Phi_n, C_1(\lambda, x_0=0)\Phi_m)(\Phi_m, C_2(\lambda', x_0'=0)\Phi_l)$$

$$\times (\Phi_l, C_3(\lambda'', x_0''=0)\Phi_n)\delta(E - E_m + E_n)\delta(E' - E_l + E_n) . \qquad \text{(IV. 3)}$$

Together with (IV. 1) we also introduce functions which in a well-defined sense are analogous to the earlier introduced retarded and advanced functions:

$$K_1(x,x',x') = \theta(t)\ \theta(t')\ K(x,x',x'') ,$$

$$K_2(x,x',x') = \theta(-t)\ \theta(-t')\ K(x,x',x'') ,$$

$$K_3(x,x',x') = -\theta(-t)\ \theta(t')\ K(x,x',x'') , \qquad \text{(IV. 4)}$$

$$K_4(x,x',x') = -\theta(t)\ \theta(-t')\ K(x,x',x'') ,$$

$$\theta(t) = 1 , \quad t > 0 , \qquad \theta(t) = 0 , \quad t < 0 .$$

Putting

$$K_i(x,x',x') = \int_{-\infty}^{+\infty} dE\, dE'\, K_i(\lambda, \lambda', \lambda''; E, E')\, e^{-iEt - iE't'} , \qquad \text{(IV. 5)}$$

$$i = 1,2,3,4 ,$$

* Bonch-Bruevich 1959a.

and dropping for the sake of convenience the arguments λ, λ', and λ'' we get

$$K_1(E,E') = \left(\frac{i}{2\pi}\right)^2 \int_{-\infty}^{+\infty} d\omega\, d\omega' \frac{J(\omega,\omega')}{(E-\omega+i\varepsilon)(E'-\omega'+i\varepsilon')},$$

$$K_2(E,E') = \left(\frac{i}{2\pi}\right)^2 \int_{-\infty}^{+\infty} d\omega\, d\omega' \frac{J(\omega,\omega')}{(E-\omega-i\varepsilon)(E'-\omega'-i\varepsilon')},$$

$$K_3(E,E') = \left(\frac{i}{2\pi}\right)^2 \int_{-\infty}^{+\infty} d\omega\, d\omega' \frac{J(\omega,\omega')}{(E-\omega-i\varepsilon)(E'-\omega'+i\varepsilon')}, \qquad \text{(IV. 6)}$$

$$K_4(E,E') = \left(\frac{i}{2\pi}\right)^2 \int_{-\infty}^{+\infty} d\omega\, d\omega' \frac{J(\omega,\omega')}{(E-\omega+i\varepsilon)(E'-\omega'-i\varepsilon')}.$$

If we consider E and E' to be complex variables, we see that $K_1(E,E')$ is an analytical function in the region Im $E > 0$, Im $E' > 0$, $K_2(E,E')$ in the region Im $E < 0$, Im $E' < 0$, and so on. The set $\{K_1, K_2, K_3, K_4\}$ can thus be considered to be one analytical function $\mathcal{K}$ of two complex variables E and E' with singularities (such as a cut) when Im $E = 0$, Im $E' = 0$. One can easily express the spectral function J in terms of the limiting values of $\mathcal{K}$ when the imaginary parts of E and E' tend to zero. We find easily from (IV. 6) that for real E and E' we have

$$\begin{aligned} J(E,E') &= \mathcal{K}(E+i\varepsilon, E'+i\varepsilon') + \mathcal{K}(E-i\varepsilon, E'-i\varepsilon') - \mathcal{K}(E-i\varepsilon, E'+i\varepsilon') \\ &\quad - \mathcal{K}(E+i\varepsilon, E'-i\varepsilon') \\ &= K_1(E,E') + K_2(E,E') - K_3(E,E') - K_4(E,E'), \qquad \text{(IV. 7)} \end{aligned}$$

$$\varepsilon, \varepsilon' > 0, \qquad \varepsilon, \varepsilon' \to 0.$$

Let us now consider the causal function

$$K_c = \langle T\{C_1(x)C_2(x')C_3(x'')\}\rangle, \qquad \text{(IV. 8)}$$

To evaluate it we need to know the spectral functions for triple products of operators in different order. Let us give the function considered earlier a superscript (1, 2, 3), and let us denote by $J^{(2,1,3)}, \ldots$ the spectral functions for the corresponding products. Using (IV. 3) one sees easily that the following relations are valid

$$J^{(2,3,1)}(E,E') = e^{\beta E'} J^{(1,2,3)}(-E', E-E'), \qquad \text{(IV. 9)}$$

$$J^{(3,1,2)}(E,E') = e^{\beta E} J^{(1,2,3)}(E'-E, -E), \qquad \text{(IV. 10)}$$

$$J^{(1,3,2)}(E,E') = e^{\beta E'} J^{(2,1,3)}(-E', E-E'), \qquad \text{(IV. 11)}$$

$$J^{(3,2,1)}(E,E') = e^{\beta E} J^{(2,1,3)}(E'-E, -E). \qquad \text{(IV. 12)}$$

The causal function (IV. 8) can thus in general be expressed in terms of two spectral functions, $J^{(1,2,3)} \equiv J_1$ and $J^{(2,1,3)} \equiv J_2$ (the second of these satisfies an equation similar to (IV. 7)). We note, however, that in the particular case where $C_2 = C_1$, and C_3 real we have $J_2 = J_1^+$.

Let us, as before, denote by η_{ij} the factor which is equal to +1 or -1 depending on whether the number of fermion operators which are permuted when we go from C_iC_j to C_jC_i, where $i,j = 1,2,3$, is even or odd. We find easily from (IV. 9) to (IV. 12)

$$K_c(x, x', x'') = \int_{-\infty}^{+\infty} dE\, dE'\, e^{-iEt - iE't'}\, K_c(\lambda, \lambda', \lambda''; E, E') \,, \quad \text{(IV. 13)}$$

where

$$\begin{aligned} K_c(E, E') = (\tfrac{i}{2\pi})^2 \int_{-\infty}^{+\infty} d\omega\, d\omega'\, J_1(\omega, \omega') \Big[& \frac{1}{(E - \omega + i\varepsilon)\,(E' - \omega' + i\varepsilon')} \\ & - \eta_{12}\,\eta_{13}\, \frac{e^{-\beta\omega}}{(E - \omega' + \omega - i\varepsilon)\,(E' - E + \omega' + i\varepsilon')} \\ & - \eta_{23}\,\eta_{13}\, \frac{e^{-\beta\omega'}}{(E - E' + \omega + i\varepsilon)\,(E' - \omega + \omega' - i\varepsilon')} \Big] \\ & - J_2(\omega, \omega') \Big[\frac{1}{(E - E' - \omega + \omega' + i\varepsilon)\,(E' - \omega' - i\varepsilon')} \\ & + \eta_{23}\, \frac{e^{-\beta\omega}}{(E - \omega' + \omega + i\varepsilon)\,(E' - E + \omega' - i\varepsilon')} \\ & - \eta_{12}\,\eta_{13}\,\eta_{23}\, \frac{e^{-\beta\omega'}}{(E + \omega' - i\varepsilon)\,(E' - \omega + \omega' - i\varepsilon')} \Big] \Big] \,. \end{aligned} \quad \text{(IV. 14)}$$

The function $K_c(E, E')$ is, of course, not an analytical one.

One can consider in a completely analogous manner also Green functions depending on n time-arguments. In thermodynamic equilibrium they depend on n-1 time-arguments, and we need introduce 2^{n-1} "retarded" and "advanced" functions K_i ($i = 1, \ldots, 2^{n-1}$). The Fourier transforms of these which can be expressed as n-1-dimensional Cauchy-type integrals are analytical functions of n-1 variables, $E_1, \ldots, E_{n-1}$ (each in the region obtained by the appropriate choice of signs of the imaginary parts of the E_i). All K_i together form one analytical function $\mathcal{K}$ which has cuts along the hypersurfaces Im $E_i = 0$ ($i = 1, \ldots, n-1$). The spectral function $J(E_1, \ldots, E_{n-1})$ can, as in (IV. 7), be expressed in terms of the limiting values of $\mathcal{K}$ when the imaginary parts of the E_i tend to zero in all possible ways.

Appendix V

THE BETHE-SALPETER EQUATION

We shall obtain in this appendix an explicit equation for the two-particle Green function

$$G_{2c}(x_1,x_2;x_1',x_2') = i\langle T\{a(x_1)a(x_2)a^+(x_1')a^+(x_2')\}\rangle$$

$$= \lim_{J\to 0} G_{2c}(x_1,x_2;x_1',x_2';J) ,$$

$$G_{2c}(x_1,x_2;x_1',x_2';J) = \frac{i}{\langle S\rangle}\langle T\{a(x_1)a(x_2)a^+(x_1')a^+(x_2')S\}\rangle , \tag{V. 1}$$

$$S = T\{\exp(i\int J(x)\,\phi(x)\,d^4x)\} .$$

We shall perform our calculations for fermion systems interacting with a quantised field. Using the results of section f of appendix I we can immediately apply the results obtained here to the case of systems with direct interactions.

We shall denote the operator occurring on the left-hand side of (8. 8) by $F(x) - i g \Gamma^{(o)}(\delta/\delta J(x))$. Using the equation of motion for $a(x)$ and proceeding as in sections 7 and 8 we find

$$\{F(x_1) - i g \Gamma^{(o)} \frac{\delta}{\delta J(x_1)}\} G_{2c}(x_1,x_2;x_1',x_2';J)$$

$$= - i \delta(x_1-x_1') G_c(x_2,x_2';J) + i \delta(x_1-x_2') G_c(x_2,x_1';J) . \tag{V. 2}$$

Hence

$$\int d^4x_2' G_c^{-1}(x_2,x_2')\{F(x_1) - i g \Gamma^{(o)} \frac{\delta}{\delta J(x_1)}\} G_{2c}(x_1,x_2;x_1',x_2')$$

$$= - i \delta(x_1-x_1')\delta(x_2-x_2') + i \delta(x_1-x_2')\delta(x_2-x_1') . \tag{V. 3}$$

It is convenient for the following to use a symbolical notation and to consider all quantities occurring in (V. 3) to be matrices. We then get from (V. 3)

$$G_2^{-1}(F_1 - i g \Gamma^{(o)} \frac{\delta}{\delta J_1}) G_{12} = - i I_{12} , \tag{V. 3a}$$

where I_{12} is the matrix with elements:

$$(x_1,x_2|I_{12}|x_1',x_2') = \delta(x_1-x_1')\delta(x_2-x_2') - \delta(x_1-x_2')\delta(x_2-x_1') .$$

The indices 1 and 2 indicate now on which variables (x_1 or x_2) the operator acts, and we have dropped the index "c" as we are dealing only with causal functions.

From (9.7) we have

$$G_1^{-1} = - F_1 + M_1 , \tag{V.4}$$

where M_1 is the mass operator. We must emphasise that the mass operator acts by definition only in the space of the dynamical variables with the appropriate index; the functional derivative in (V.3), on the other hand, acts, of course, upon functions of any arguments. The operators $i g \Gamma^{(o)}(\delta/\delta J)$ and M_1 are thus the same only in the function space where the arguments have one index only; in the case considered at the present moment they need not be identical. We write therefore the second factor on the left-hand side of (V.3a) as follows

$$F_1 - i g \Gamma^{(o)} \frac{\delta}{\delta J} = - G_1^{-1} + M_1 - i g \Gamma^{(o)} \frac{\delta}{\delta J} , \tag{V.5}$$

and we get thus from (V.3a)

$$G_2^{-1}(G_1^{-1} - M_1 + i g \Gamma^{(o)} \frac{\delta}{\delta J}) G_{12} = i I_{12} . \tag{V.6}$$

On the other hand, we can always write

$$(G_1^{-1} G_2^{-1} - V_{12}) G_{12} = i I_{12} , \tag{V.7}$$

where the operator V_{12} is defined by this equation. It is clear that it describes the interaction between the particles, as G_{12} is equal to the antisymmetrised product $G_1 G_2$ (apart from a factor i) when there are no interactions. If we express the product $V_{12} G_{12}$ in terms of Green functions and vertex parts, we shall obtain an equation such as (9.7) for G_{12}, and that is our present aim.

Comparing (V.6) and (V.7) we get

$$\begin{aligned} V_{12} G_{12} &= - i g G_2^{-1} \Gamma^{(o)} \frac{\delta G_{12}}{\delta J} + G_2^{-1} M_1 G_{12} \\ &= G_2^{-1} M_1 G_{12} - i g \Gamma^{(o)} \frac{\delta}{\delta J}(G_2^{-1} G_{12}) + i g \Gamma^{(o)} \frac{\delta G_2^{-1}}{\delta J} G_{12} . \end{aligned}$$

It follows from (V.7) that

$$\frac{\delta}{\delta J}(G_2^{-1} G_{12}) = G_1 \frac{\delta}{\delta J}(V_{12} G_{12}) - G_1 \frac{\delta G_1^{-1}}{\delta J} G_2^{-1} G_{12} ,$$

and thus

$$\begin{aligned} V_{12} G_{12} = G_2^{-1} M_1 G_{12} &+ i g \Gamma^{(o)} \frac{\delta G_2^{-1}}{\delta J} G_{12} - i g \Gamma^{(o)} G_1 \frac{\delta}{\delta J}(V_{12} G_{12}) \\ &+ i g \Gamma^{(o)} \frac{\delta G_1^{-1}}{\delta J} G_2^{-1} G_{12} . \end{aligned} \tag{V.8}$$

From (9.5) and (9.4) it follows that

$$M_1 = - i g \Gamma^{(o)} G_1 \frac{\delta G_1^{-1}}{\delta J} ,$$

and the first and last term on the right-hand side of (V. 8) cancel one another. The second term on the right-hand side of (V. 8) can be rewritten as follows:

$$i g \Gamma^{(o)} \frac{\delta G_2^{-1}}{\delta J} G_{12} = i g^2 \Gamma_1^{(o)} \Gamma_2 D_2' G_{12} ,$$

and we have thus

$$V_{12} G_{12} = i g^2 \Gamma_1^{(o)} \Gamma_2 D_2' G_{12} - i g \Gamma_1^{(o)} G_1 \frac{\delta}{\delta J} (V_{12} G_{12}) . \qquad (V. 9)$$

This is an equation for $V_{12}G_{12}$ which one can solve by iteration, for instance. In the first approximation, in particular, we can drop the second term and get

$$V_{12} G_{12} \cong i g^2 \Gamma_1^{(o)} \Gamma_2^{(o)} D_2' G_{12} , \qquad (V. 10)$$

or, if we display all arguments explicitly,

$$\int d^4x_3 \, d^3x_4 \, V_{12}(x_1, x_2; x_3, x_4) \, G_{2c}(x_3, x_4; x_1', x_2')$$
$$= i g^2 \Gamma_1^{(o)} \Gamma_2^{(o)} D_c'(x_1, x_2) \, G_{2c}(x_1, x_2; x_1', x_2') . \qquad (V. 10a)$$

We then get from (V. 7)

$$\int G_c^{-1}(x_1, x') \, G_c^{-1}(x_2, x'') \, G_{2c}(x', x''; x_1', x_2') \, d^4x' \, d^4x''$$
$$- i g^2 \Gamma_1^{(o)} \Gamma_2^{(o)} D_c'(x_1, x_2) \, G_{2c}(x_1, x_2; x_1', x_2')$$
$$= i \delta(x_1 - x_1') \, \delta(x_2 - x_2') - i \delta(x_1 - x_2') \, \delta(x_2 - x_1') . \qquad (V. 11)$$

It is apparently most convenient to use as boundary conditions for (V. 11) the requirement that G_{2c} can be written in the form (IV. 14).

We obtained (V. 7) - and thus (V. 11) - for arbitrary temperatures. For $T = 0$ it becomes the equation for bound states which is well known in quantum field theory (Salpeter and Bethe 1951, Gell-Mann and Low 1951, Schwinger 1951, Polivanov 1954). In particular, if we replace in (V. 11), in the spirit of the approximation (V. 10), G_c and D_c' by $G_c^{(o)}$ and $D_c^{(o)}$ we get the so-called Bethe-Salpeter equation which Salpeter and Bethe (1951) introduced in quantum electrodynamics. One can easily give a diagrammatical description of this equation, using the rules from appendix I. The function G_{2c} satisfying this equation is the result of summing the diagrams shewn in Fig. 9. Such diagrams are sometimes called "ladder" diagrams, and the approximation (V. 10) is accordingly called the "ladder" approximation.

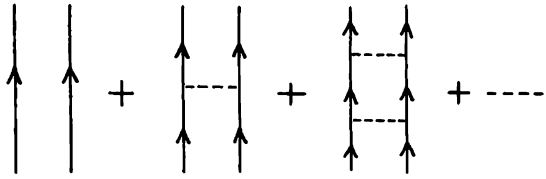


Fig. 9.

We can use (I. 62) to apply (V. 11) immediately to the case of systems with direct interactions: we need only make the following substitution in the second term on the left-hand side:

$$g^2 \, D_c^{(0)}(x_1, x_2) \to \delta(x_{1,0} - x_{2,0}) \; U(\vec{x}_1 - \vec{x}_2). \tag{V.12}$$

One can also easily obtain equations such as (V. 7) or (V. 11) for boson systems. Indeed, the antisymmetrical properties of G_{2c} were only once used explicitly, namely when writing down the right-hand side of (V. 3). It follows thus that one only need change the sign of the second term on the right-hand sides of (V. 7) and (V. 11) to get the formulae for the boson case.

Appendix VI

THE MASS OPERATOR AND VERTEX PART FOR SYSTEMS WITH DIRECT INTERACTIONS

We can introduce a mass operator and vertex part for systems with direct binary interactions in complete analogy with the case discussed in section 9 where the interaction was assumed to be through a field. It is convenient to work in the coordinate representation, using the equations of section 8. To simplify the equations we shall introduce the quantities

$$U'(x-x'') = U(\vec{x}-\vec{x}'')\ \delta(x_0-x_0'')\ , \tag{VI. 1}$$

$$F'(x,x') = F(\vec{x},\vec{x}')\ \delta(x_0-x_0')\ , \tag{VI. 2}$$

$$\Psi(x,x') = -\,i\,\frac{\delta \ln \langle S\rangle}{\delta F'(x,x')}\,. \tag{VI. 3}$$

We have then

$$S = T\{\exp[i\int d^4z\, d^4z'\, F'(z,z')\ a^+(z)\ a(z')\}\ , \tag{VI. 4}$$

and we get from (8. 23a)

$$\{i\frac{\partial}{\partial x_0} + \mu - T_{\vec{x}} - V(\vec{x})\}\ G_c(x,x') + \int d^4x''\ F'(x,x'')\ G_c(x'',x')$$

$$-\tfrac{1}{2}\int d^4x''\, U'(x-x'')\ \{-\,i\,\frac{\delta G_c(x,x')}{\delta F'(x'',x'')} \pm i\,\frac{\delta G_c(x'',x')}{\delta F'(x'',x)} + G_c(x,x')\ \Psi(x'',x'')$$

$$\mp\ G_c(x'',x')\ \Psi(x'',x)\} = -\,\delta(x-x')\ . \tag{VI. 5}$$

To simplify our equations we have not explicitly indicated the functional dependence of G_c on F'; the upper (lower) signs refer to fermions (bosons).

As in section 9 we shall change the functional argument, and put

$$\frac{\delta G_c(x'',x')}{\delta F'(x'',x)} = -\int d^4u\, d^4v\, d^4z\, d^4z'\ G_c(x'',u)\ \frac{\delta G_c^{-1}(u,v)}{\delta \Psi(z,z')}$$

$$\times\ G_c(v,x')\ \frac{\delta \Psi(z,z')}{\delta F'(x'',x)}\,. \tag{VI. 6}$$

We introduce the notation

$$\frac{\delta G_c^{-1}(u, v)}{\delta \Psi(z, z')} = \Gamma(u, v; z, z') , \tag{VI. 7}$$

$$\frac{\delta \Psi(z, z')}{\delta F'(x'', x)} = D(z, z'; x'', x) . \tag{VI. 8}$$

The quantities defined by (VI. 7) and (VI. 8) are clearly analogous to the vertex part and field Green function - as is indicated in their notation. It will become clear in the following that this is not merely a formal analogy but that it has a deeper meaning: D turns out to be connected with the two-particle Green function (5. 24) the poles of which describe - as we know - the "pair" excitations of the system.

Using (VI. 6) to (VI. 8) we can write (VI. 5) in the form

$$\{i \frac{\partial}{\partial x_0} + \mu - T_{\vec{x}} - V(\vec{x})\} G_c(x, x') + \int d^4x'' F'(x, x'') G_c(x'', x') - \int d^4y M(x, y) G_c(y, x') = - \delta(x-x') , \tag{VI. 9}$$

where the mass operator $M(x, y)$ is defined by the equation

$$M(x, y) = \frac{i}{2} \int d^4x'' d^4z d^4z' d^4z'' U'(x-x'') \{G_c(x, z) \Gamma(z, y; z', z'') \times D(z', z''; x'', x'') - G_c(x'', z) \Gamma(z, y; z', z'') D(z', z''; x'', x)\} - \tfrac{1}{2} U'(x;y) \Psi(y, x) + \tfrac{1}{2} \int d^4x'' U'(x-x'') \Psi(x'', x'') \delta(x-y) . \tag{VI. 10}$$

This way of writing down the mass operator is convenient if we wish to solve (VI. 9) by iteration using the method of section 11. Let us first of all obtain the first approximation for the "vertex part" assuming formally that U' is proportional to some small parameter ϵ. This operation is as in section 11 purely formal; in practice one can only find the expansion parameter by using the renormalisation group method. Taking the matrix product of (VI. 9) and G_c^{-1} we get

$$\{i \frac{\partial}{\partial x_0} + \mu - T_{\vec{x}} - V(\vec{x})\} \delta(x-x') - M(x, x') + F'(x, x') = - G_c^{-1}(x, x') ,$$

and hence, using (VI. 7) and (VI. 10)

$$\Gamma(u, v; z, z') = \tfrac{1}{2}\{U'(u-v) \delta(v-z) \delta(u-z') - U'(u-z') \delta(z-z') \delta(u-v)\} - \frac{\delta F'(u, v)}{\delta \Psi(z, z')} + O(\epsilon^2) . \tag{VI. 11}$$

Furthermore, we get for D by performing the variation in (VI. 8) and (VI. 3) explicitly and afterwards putting $F' = 0$:

$$D(z, z'; x'', x) = - i \{<T [a^+(z)a(z')a(x)a^+(x'')> - G_c(x, x'') G_c(z', z)\} . \quad \text{(VI. 12)}$$

By virtue of (VI. 1) and (VI. 2) we have practically always $z'_0 = z_0$ and $x''_0 = x_0$ so that the first term within the braces is closely connected with (5. 24) as we noted earlier.

It follows from (VI. 12) that the introduction of the mass operator does not relieve us of the necessity to determine some kind of two-particle Green function. In other words, (VI. 9) shares the fate of (7. 7) of not being a "closed" equation *. There is, however, a difference in the actual form of the two-particle Green functions occurring in these equations; this may turn out to be important when we want to apply some kind of approximate method for solving them.

From the definition (VI. 8) it follows that

$$\int \frac{\delta F'(u, v)}{\delta \Psi(z, z')} D(z, z'; y, y') \, d^4z \, d^4z' = \delta(u-y) \, \delta(v-y') . \quad \text{(VI. 13)}$$

Moreover, in zeroth approximation we have

$$D(z, z'; x'', x) = - i \, G_c(z', x'') \, G_c(x, z) .$$

We see from (VI. 10), (VI. 11), and (VI. 13) that the mass operator in first approximation is given by the formula

$$M_1(x, y) = - \int d^4x'' \, U'(x-x'') \{\delta(x''-y) \, \Psi(x'', x) - \delta(x-y) \, \Psi(x'', x'')\} . \quad \text{(VI. 14)}$$

Using (VI. 1) and (8. 24a), and denoting as everywhere the average particle concentration at $\vec{x}$ by $n(\vec{x})$ we get finally

$$M_1(x, y) = - \{U(\vec{x}-\vec{y}) \, \rho_1(\vec{y}, \vec{x}; x_0) - \int d^3\vec{x}' \, U(\vec{x}-\vec{x}') \, n(\vec{x}') \, \delta(\vec{x}-\vec{y})\} \, \delta(x_0-y_0) . \quad \text{(VI. 15)}$$

We must evaluate ρ_1 and n here using the zeroth approximation Green functions.

In the second approximation the mass operator consists of two terms

$$M_2(x, y) = M'_2(x, y) + M''_2(x, y) . \quad \text{(VI. 16)}$$

The first term M'_2 is obtained by iterating (VI. 15) where we take now for ρ_1 and n the results of the first approximation. The second term M''_2 derives from the first term on the right-hand side of (VI. 11) and is of the form

* This is, of course, also true for systems of particles interacting through a field: in the equation for G_c the field Green function D_c occurs.

$$M_2(x, y) = -\int d^3\vec{z}\, d^3\vec{z}'\, U(\vec{x}-\vec{z})\, U(\vec{y}-\vec{z}')$$

$$\times \{G\ (\vec{x}, x_0; \vec{z}', y_0)\, G_c(\vec{z}', y_0; \vec{z}, x_0)\, G_c(\vec{z}, x_0; \vec{y}, y_0)$$

$$- G_c(\vec{z}, x_0; \vec{z}', y_0)\, G_c(\vec{z}', y_0; \vec{z}, x_0)\, G_c(\vec{x}, x_0; \vec{y}, y_0)\}. \quad \text{(VI. 17)}$$

Here we must take for G_c the zeroth approximation function, that is, the one evaluated for the case where there are no interactions.

Appendix VII

RECENT DEVELOPMENTS *

Professors Bonch-Bruevich and Tyablikov state in their foreword to the present English edition that bringing the present volume up-to-date would require a second volume. We shall therefore only briefly survey recent progress mentioning mainly those topics covered in the foregoing. This means, for instance, that we shall not discuss applications of Green function methods to nuclei or in Hartree-Foc.. theory.

A number of papers have appeared dealing with general aspects of Green function theory. We may mention here the work by Ezawa, Tomozwa, and Umezawa (1957) on the quantum statistics of fields, by Migdal (1959) who extended Gor'kov's considerations (1958) to finite systems, by Balian and De Dominicis (1960) on general properties, by McCumber (1960) on sound waves, by Watanabe, Kamei, and Ezawa (1961) on field theoretical aspects of Green function methods, and by Kobe (1962) on the spectral representation of many-time Green functions. We may also draw attention to a number of general surveys, such as Thouless' book (1961) and the article by Alekseev (1961) (see also Pines 1961) which have sections on Green function methods, or survey articles devoted to Green functions such as the ones by Fradkin (1959e), Kato, Kobayashi, and Namiki (1960), Baym and Mermin (1961), Maleev (1961), Ashby (1961), and ter Haar (1962).

Functional derivative methods have been discussed by Kobelev (1958a, b, c, d, e, 1959), Fradkin (1959c, d) and Engelberg (1962). An interesting development has been the combination of functional derivative and path integration methods (Feynman 1948; for a survey of this subject see Brush 1961) by Kobelev (1960, 1961a).

Bolsterli (1960) and ter Haar and Parry (1962) have drawn attention to the fact that it is necessary to choose with care the Green functions, the poles of which are to be used for a determination of the excitation energy spectrum.

Van Hove (1954) (see also Elliott and Marshall (1958)) has discussed the close relationship between correlation functions and neutron-scattering cross-sections. Often the most convenient method for evaluating correlation functions is by computing the corresponding Green functions. This topic has been discussed in general

* This appendix was added by the translator.

terms by Baym (1961a) and Izyumov (1961); Kashcheev and Krivoglaz (1961) have considered the influence of anharmonicity on neutron-scattering cross-sections while Pitaevskii (1959) and Parry and Turner (1962) have discussed neutron-scattering by liquid helium. In this connexion we may also mention the work of Suris (1961) on helium three and by Balian and De Dominicis (1960) on Fermi liquids.

Baym and Kadanoff (1961; see also Baym 1962) have discussed in great detail the general application of Green function methods to the theory of transport phenomena (compare also Kubo 1957 and the discussion in chapter III) while Klinger (1961) discussed transport phenomena in a strong magnetic field.

The literature on superconductivity is growing fast and among the papers applying Green function methods we mention those by Eliashberg (1960), Zubarev (1960a), Kadanoff and Martin (1961), Tolmachev (1961a), Sawicki (1961), Ambegaokar and Kadanoff (1961), Valatin (1962), and Engelsberg (1962). Galitskiĭ (1958a) and Tsekhmistrenko (1959) have considered sound waves in superconductors, while Abrikosov, Gor'kov, and Khalatnikov (1958) discussed superconductivity in a high-frequency field; Morel and Anderson (1962) have considered the possibility of replacing the BCS potential by a more realistic one.

Among the papers on plasmas and the electron gas we mention those by Tareeva (1960), Kanazawa and Watabe (1960), Kanazawa, Misawa, and Fujita (1960), Akhiezer and Peletminskiĭ (1960), Mironov (1961), Tzoar and Klein (1961), Pargamanik (1961), and Glick (1962). Plasmas in solids have been discussed by Buikov (1960), Falk (1960), and Baym (1961b), while Abrikosov (1961) discussed the properties of highly condensed matter. Among papers discussing Green function techniques applied to solid state problems we may mention those by Kanazawa and Matsudaira (1960) and by Ichimura and Tanaka (1960) on diamagnetism, by Bonch-Bruevich and Mironov (1961) on the influence of impurities on the electron energy-spectrum, by Dzyub (1960) on excitons, by Tyablikov and Moskalenko (1961a, b) on polarons and F-centers, by Anderson (1961) who reduced the problem of localised magnetic states in certain metals to an exactly soluble problem strongly reminiscent of the BCS model of superconduvtivity, and by Engelsberg (1961) and Tsytovich (1962) on the loss of energy on passage through plasmas or dielectrics.

In ferromagnetism Izyumov and Yakovlev (1960) and Kawasaki and Mori (1961a, b) have extended the Bogolyubov-Tyablikov theory (see chapter VII) to higher spin-values. Their method has been criticised by Tahir-Kheli (1962, Tahir-Kheli and ter Haar 1962a) who tackled the same problem by a better method. Tahir-Kheli (1962, Tahir-Kheli and ter Haar 1962b, c, d) also discussed the influence of higher-order decoupling, the various mechanisms leading to finite line-widths in ferromagnetic resonance, and various aspects

of neutron-scattering by ferromagnetics. Ferromagnetic resonance is discussed by Tyablikov and Fu-Cho (1961), while a paper by Fu-Cho (1961) deals with antiferromagnetic resonance. Vonsovskii and Izyumov (1960) consider ferromagnetism in transition metals and Vonsovskii and Kobelev (1961) the collective model of ferromagnetism. Other papers in this field are by Fu-Cho, Tyablikov, and Shiklosh (1960), Tyablikov and Shiklosh (1960), Kobelev (1961a, b), Potapkov and Tyablikov (1960), and Izyumov and Polyak (1960).

We must finally refer to some papers dealing with the use of Green function methods in perturbation theory. Tolmachev (1961b) has discussed perturbation theory applied to an imperfect fermion system, ter Haar (1961b) has shewn how the Green function equations of motion naturally lead to the Brillouin-Wigner perturbation theory expansion, and ter Haar and Wergeland (1961) have shewn how the same equations of motion can be used to obtain the Weisskopf-Wigner expression for the natural line-width of a spectral line. Finally we must refer to an interesting and important study by Tyablikov and Bonch-Bruevich (1962) devoted to perturbation theoretical aspects of the temperature-dependent Green functions *. They discuss at some length the advantage of not expanding the Green functions, but their inverse in a power series in some small parameter. The connexion with Hartree-Fock theory is considered, and also the problem of expressing the mass operator in terms of the scattering amplitude.

* Unfortunately this study became available too late to be incorporated in its entirety, as it deserved to be.

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We have used the following abbreviations: JETP: Journal of Experimental and Theoretical Physics (U.S.S.R.); UFN: Uspekhi Fizicheskikh Nauk (U.S.S.R.); DAN: Doklady Akad. Nauk SSSR; FTT: Solid State Physics (U.S.S.R.); FMM: Physics of Metals and Metallography (U.S.S.R.); SP: indicates the English translation of the Russian original publihed by the American Institute of Physics in their Soviet Physics series which includes Soviet Physics JETP, Soviet Physics Uspekhi, Soviet Physics Doklady, and Soviet Physics Solid State. FMM is also translated from cover to cover, but we have not given the references to the translations, as they follow the pagination of the original closely. Other abbreviations follow the Style Manual of the American Institute of Physics.

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